



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 4WNU / pdb_00004wnu
Title : Human Cytochrome P450 2D6 Quinidine Complex
Authors : Wang, A.; Stout, C.D.; Johnson, E.F.
Deposited on : 2014-10-14
Resolution : 2.26 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

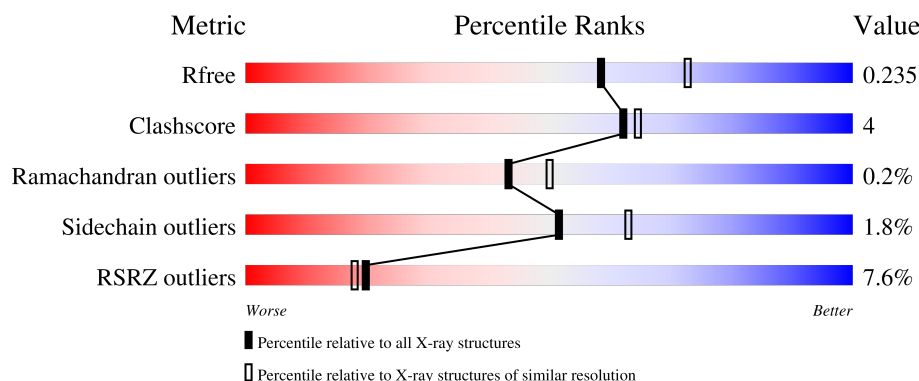
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	479	5% 85% 8% 6%
1	B	479	8% 85% 10% 5%
1	C	479	8% 86% 7% 6%
1	D	479	7% 80% 13% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15307 atoms, of which 0 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 Cytochrome P450 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3553	2276	630	633	14			
1	B	453	Total	C	N	O	S	0	0	0
			3591	2302	637	638	14			
1	C	452	Total	C	N	O	S	0	0	0
			3575	2290	635	636	14			
1	D	450	Total	C	N	O	S	0	0	0
			3570	2288	633	635	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	initiating methionine	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635

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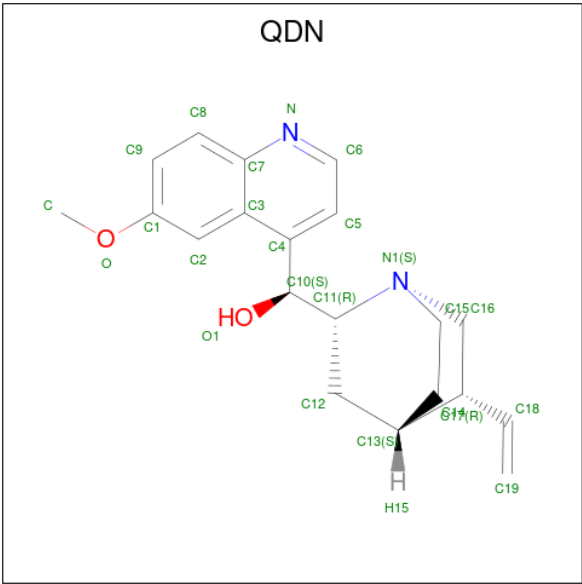
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	23	MET	-	initiating methionine	UNP P10635
C	24	ALA	-	expression tag	UNP P10635
C	25	LYS	-	expression tag	UNP P10635
C	26	LYS	-	expression tag	UNP P10635
C	27	THR	-	expression tag	UNP P10635
C	28	SER	-	expression tag	UNP P10635
C	29	SER	-	expression tag	UNP P10635
C	30	LYS	-	expression tag	UNP P10635
C	31	GLY	-	expression tag	UNP P10635
C	32	LYS	-	expression tag	UNP P10635
C	33	LEU	-	expression tag	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	23	MET	-	initiating methionine	UNP P10635
D	24	ALA	-	expression tag	UNP P10635
D	25	LYS	-	expression tag	UNP P10635
D	26	LYS	-	expression tag	UNP P10635
D	27	THR	-	expression tag	UNP P10635
D	28	SER	-	expression tag	UNP P10635
D	29	SER	-	expression tag	UNP P10635
D	30	LYS	-	expression tag	UNP P10635
D	31	GLY	-	expression tag	UNP P10635
D	32	LYS	-	expression tag	UNP P10635
D	33	LEU	-	expression tag	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635
D	501	HIS	-	expression tag	UNP P10635

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



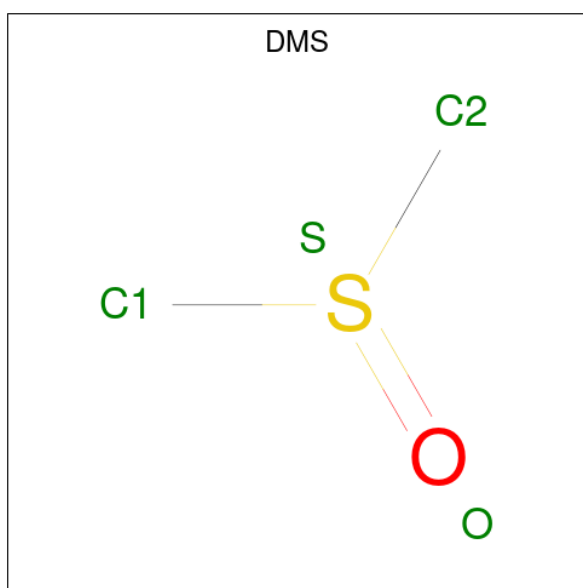
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is Quinidine (CCD ID: QDN) (formula: C₂₀H₂₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		
3	C	1	Total	C	N	O	0	0
			24	20	2	2		
3	D	1	Total	C	N	O	0	0
			24	20	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

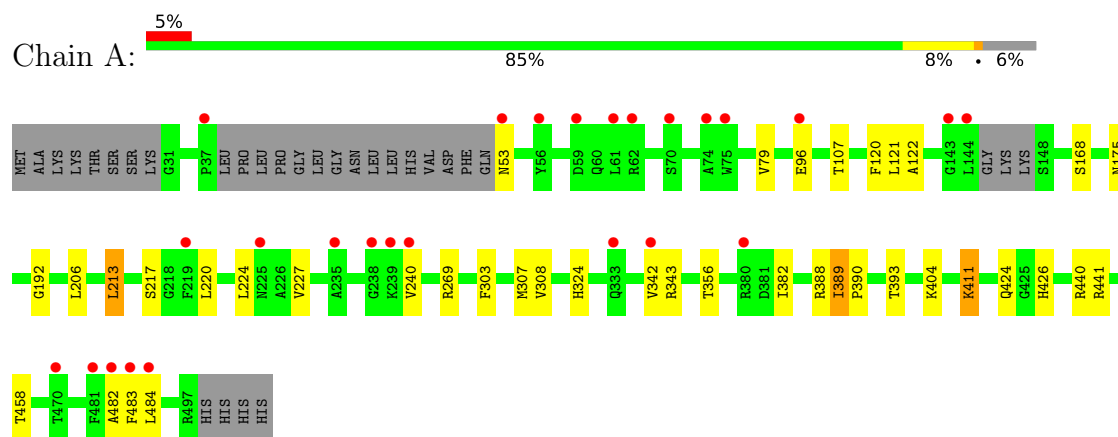
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	201	Total	O	0	0
			201	201		
7	B	174	Total	O	0	0
			174	174		
7	C	186	Total	O	0	0
			186	186		
7	D	108	Total	O	0	0
			108	108		

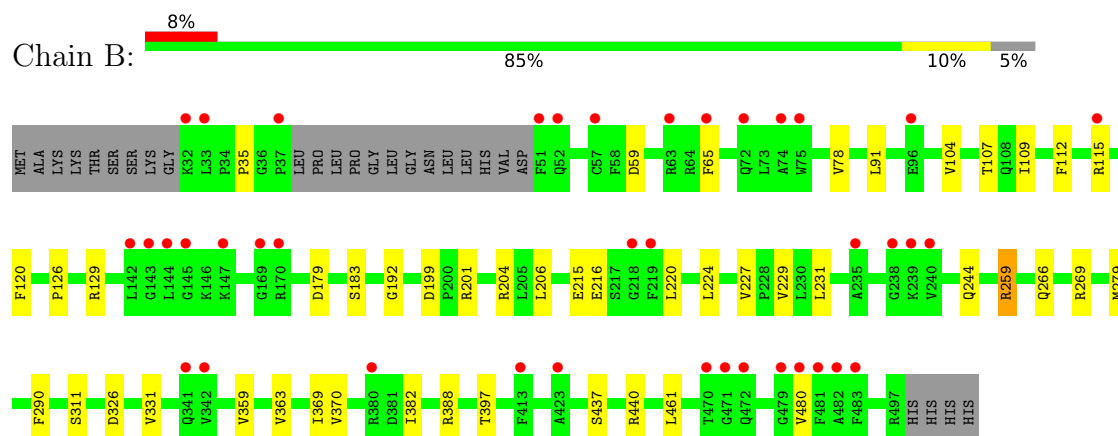
3 Residue-property plots [i](#)

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.

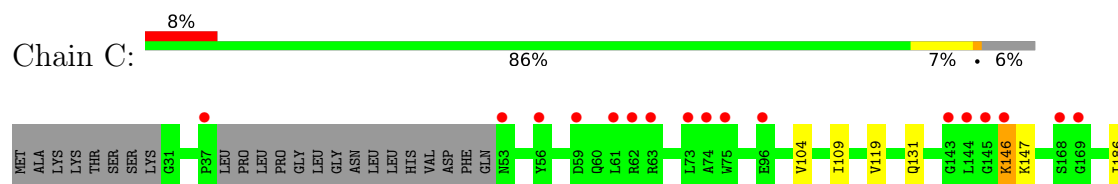
• Molecule 1: Cytochrome P450 2D6

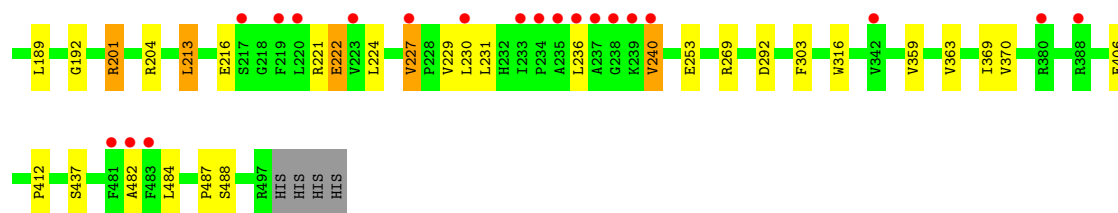


• Molecule 1: Cytochrome P450 2D6

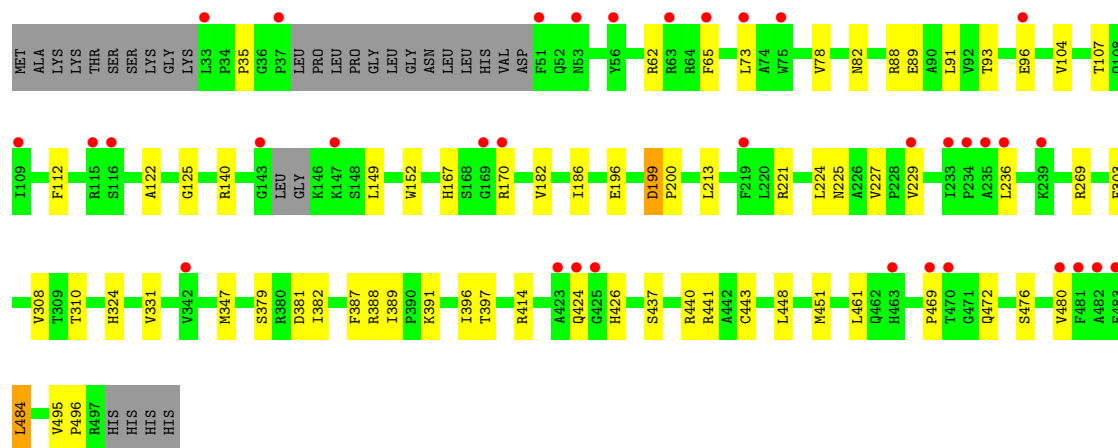
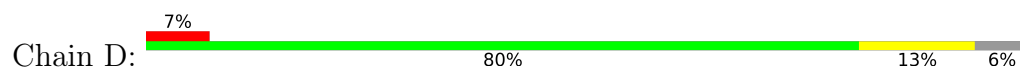


• Molecule 1: Cytochrome P450 2D6





● Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.34Å 192.11Å 250.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.04 – 2.26 38.04 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.04-2.26) 98.4 (38.04-2.26)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.27Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.232 0.195 , 0.235	Depositor DCC
R_{free} test set	6492 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15307	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.48 % 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 6.9501e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GOL, DMS, ZN, QDN

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	0.56	0/3647	0.85	4/4958 (0.1%)
1	B	0.49	0/3687	0.80	2/5011 (0.0%)
1	C	0.53	0/3670	0.81	2/4988 (0.0%)
1	D	0.48	0/3665	0.80	6/4981 (0.1%)
All	All	0.52	0/14669	0.81	14/19938 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ASP	CA-C-N	7.32	126.86	119.24
1	D	199	ASP	C-N-CA	7.32	126.86	119.24
1	B	199	ASP	CA-C-N	5.83	125.31	119.24
1	B	199	ASP	C-N-CA	5.83	125.31	119.24
1	D	125	GLY	CA-C-N	5.67	125.14	119.24
1	D	125	GLY	C-N-CA	5.67	125.14	119.24
1	C	227	VAL	CA-C-N	5.57	125.24	119.56
1	C	227	VAL	C-N-CA	5.57	125.24	119.56
1	A	324	HIS	CA-C-N	5.52	125.19	119.56
1	A	324	HIS	C-N-CA	5.52	125.19	119.56
1	D	324	HIS	CA-C-N	5.18	124.97	119.28
1	D	324	HIS	C-N-CA	5.18	124.97	119.28
1	A	411	LYS	CA-C-N	5.02	124.68	119.56
1	A	411	LYS	C-N-CA	5.02	124.68	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3553	0	3530	22	0
1	B	3591	0	3574	27	0
1	C	3575	0	3560	28	0
1	D	3570	0	3546	40	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	24	0	24	2	0
3	B	24	0	24	1	0
3	C	24	0	24	0	0
3	D	24	0	24	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	24	0	32	3	0
6	B	6	0	8	3	0
6	C	12	0	16	3	0
6	D	18	0	24	4	0
7	A	201	0	0	2	0
7	B	174	0	0	4	0
7	C	186	0	0	2	0
7	D	108	0	0	3	0
All	All	15307	0	14530	119	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 4.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG11	6:B:605:GOL:H11	1.60	0.83
1:D:140:ARG:NH1	7:D:780:HOH:O	2.23	0.71
1:C:224:LEU:HD21	1:C:236:LEU:HB3	1.70	0.71
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.78	0.66
1:C:146:LYS:HD2	1:C:147:LYS:HB2	1.79	0.65
1:B:369:ILE:HG13	1:B:370:VAL:HG23	1.78	0.65
1:B:91:LEU:HD11	1:B:397:THR:HG21	1.78	0.65
1:D:388:ARG:NH2	7:D:763:HOH:O	2.24	0.63
1:A:121:LEU:HD21	6:A:607:GOL:H32	1.82	0.62
1:C:224:LEU:HD23	1:C:231:LEU:HD23	1.81	0.61
1:D:122:ALA:O	1:D:441:ARG:NH2	2.18	0.60
1:C:192:GLY:O	1:C:269:ARG:NH2	2.35	0.58
1:B:388:ARG:NH1	7:B:850:HOH:O	2.33	0.58
1:D:186:ILE:HG21	1:D:303:PHE:HA	1.87	0.57
1:A:79:VAL:HG23	1:A:393:THR:HG21	1.86	0.57
1:A:175:ASN:HD22	1:A:175:ASN:H	1.51	0.56
1:C:119:VAL:HG22	1:C:131:GLN:HB3	1.86	0.56
1:C:221:ARG:HG3	1:C:222:GLU:H	1.71	0.56
1:C:221:ARG:HG3	1:C:222:GLU:N	2.21	0.56
1:D:227:VAL:HG12	1:D:229:VAL:HG12	1.88	0.56
1:A:175:ASN:OD1	6:A:609:GOL:H11	2.05	0.54
1:C:227:VAL:HG12	1:C:229:VAL:HG12	1.89	0.54
1:D:381:ASP:OD1	1:D:391:LYS:N	2.38	0.54
1:A:96:GLU:OE1	1:A:440:ARG:NH1	2.41	0.54
1:D:73:LEU:HD13	6:D:607:GOL:H2	1.88	0.54
1:B:115:ARG:HH12	1:B:126:PRO:HB2	1.72	0.53
1:A:175:ASN:H	1:A:175:ASN:ND2	2.07	0.53
1:B:440:ARG:NE	7:B:823:HOH:O	2.40	0.53
1:D:221:ARG:NH2	6:D:605:GOL:H11	2.23	0.53
1:C:224:LEU:HD22	1:C:240:VAL:HG21	1.91	0.53
2:D:601:HEM:HMB2	2:D:601:HEM:HBB2	1.90	0.52
1:B:227:VAL:HG12	1:B:229:VAL:HG12	1.91	0.52
1:C:146:LYS:CE	1:C:269:ARG:HD2	2.40	0.51
1:B:437:SER:HB3	2:B:601:HEM:HBA1	1.91	0.51
1:C:406:GLU:HA	1:C:412:PRO:HG3	1.92	0.51
1:A:192:GLY:O	1:A:269:ARG:NH2	2.42	0.51
1:C:104:VAL:HG11	6:C:605:GOL:H11	1.92	0.51
1:A:388:ARG:NH2	1:A:390:PRO:HG3	2.27	0.50
1:C:359:VAL:O	1:C:363:VAL:HG23	2.12	0.49
1:C:204:ARG:NE	7:C:835:HOH:O	2.44	0.49
1:D:152:TRP:HZ2	1:D:269:ARG:HH22	1.60	0.49
1:D:224:LEU:HD21	1:D:236:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:VAL:HG11	6:D:605:GOL:H12	1.95	0.49
1:C:316:TRP:CD1	1:C:487:PRO:HD3	2.47	0.49
1:D:382:ILE:HG13	1:D:389:ILE:HB	1.95	0.49
1:B:109:ILE:HD11	1:B:231:LEU:HD22	1.94	0.49
1:C:186:ILE:HG21	1:C:303:PHE:HA	1.95	0.49
1:C:216:GLU:OE2	6:C:605:GOL:O1	2.28	0.48
1:D:91:LEU:HD11	1:D:397:THR:HG21	1.95	0.48
1:D:88:ARG:NH1	7:D:753:HOH:O	2.46	0.48
1:D:149:LEU:HD13	1:D:448:LEU:HD13	1.96	0.48
1:B:331:VAL:HG11	1:B:461:LEU:HD12	1.95	0.48
1:C:201:ARG:HD2	1:C:253:GLU:OE2	2.15	0.47
1:D:167:HIS:O	1:D:170:ARG:HB2	2.15	0.47
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.95	0.47
1:B:129:ARG:HD2	7:B:701:HOH:O	2.14	0.47
1:A:213:LEU:HD21	1:A:308:VAL:HG21	1.96	0.47
1:C:146:LYS:HE2	1:C:269:ARG:HD2	1.96	0.46
1:A:122:ALA:O	1:A:441:ARG:NH2	2.31	0.46
1:B:35:PRO:HB2	1:B:65:PHE:HD2	1.80	0.46
1:B:215:GLU:OE1	1:B:244:GLN:HG3	2.15	0.46
1:D:443:CYS:HB2	2:D:601:HEM:NA	2.29	0.46
1:C:292:ASP:OD1	7:C:826:HOH:O	2.21	0.46
1:B:216:GLU:OE2	6:B:605:GOL:H32	2.16	0.45
1:A:342:VAL:HG13	1:A:343:ARG:H	1.81	0.45
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.87	0.45
1:A:213:LEU:HD12	3:A:602:QDN:H19	1.98	0.45
1:B:216:GLU:OE1	6:B:605:GOL:O1	2.33	0.45
1:D:107:THR:HB	1:D:112:PHE:CD2	2.52	0.45
1:D:107:THR:HB	1:D:112:PHE:CG	2.52	0.45
1:D:221:ARG:HH21	6:D:605:GOL:H11	1.81	0.44
1:D:469:PRO:HG2	1:D:472:GLN:OE1	2.17	0.44
1:D:424:GLN:HB2	1:D:426:HIS:ND1	2.33	0.44
1:A:424:GLN:HG2	1:A:426:HIS:CE1	2.53	0.44
1:B:179:ASP:OD1	1:B:311:SER:OG	2.29	0.44
1:B:183:SER:OG	1:B:206:LEU:HD21	2.17	0.44
1:B:204:ARG:NE	7:B:806:HOH:O	2.40	0.44
1:D:308:VAL:HG22	1:D:484:LEU:HD22	2.00	0.44
1:D:96:GLU:OE1	1:D:440:ARG:NH1	2.50	0.44
1:D:221:ARG:O	1:D:225:ASN:HB2	2.18	0.43
1:B:326:ASP:N	1:B:326:ASP:OD1	2.50	0.43
1:A:356:THR:HG21	1:A:458:THR:HG22	2.01	0.43
1:D:35:PRO:HD3	1:D:387:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ILE:O	1:C:484:LEU:HB2	2.18	0.43
1:D:347:MET:HG3	1:D:451:MET:HE2	2.00	0.43
1:B:359:VAL:O	1:B:363:VAL:HG23	2.19	0.43
1:A:483:PHE:CD2	1:A:484:LEU:HD13	2.53	0.43
1:D:89:GLU:O	1:D:93:THR:HB	2.19	0.43
1:A:220:LEU:O	1:A:224:LEU:HG	2.18	0.43
1:B:279:MET:HG3	1:B:290:PHE:O	2.19	0.43
1:D:213:LEU:HD11	1:D:308:VAL:HG11	2.01	0.43
1:B:107:THR:HB	1:B:112:PHE:CG	2.54	0.43
1:D:35:PRO:HB2	1:D:65:PHE:HD2	1.84	0.42
1:C:221:ARG:NH1	6:C:605:GOL:O2	2.46	0.42
1:D:331:VAL:HG11	1:D:461:LEU:HD12	2.01	0.42
1:A:440:ARG:HD2	7:A:754:HOH:O	2.19	0.42
1:A:404:LYS:NZ	7:A:834:HOH:O	2.52	0.42
1:C:227:VAL:HB	1:C:230:LEU:HD13	2.02	0.42
1:D:495:VAL:HA	1:D:496:PRO:HD3	1.77	0.42
1:D:104:VAL:HG13	1:D:225:ASN:HD21	1.83	0.42
1:A:303:PHE:HB3	1:A:307:MET:HE2	2.02	0.42
1:D:437:SER:HB3	2:D:601:HEM:HBA1	2.00	0.42
1:A:120:PHE:CE2	3:A:602:QDN:H11	2.55	0.41
1:B:220:LEU:O	1:B:224:LEU:HG	2.21	0.41
1:D:149:LEU:HD23	1:D:149:LEU:HA	1.86	0.41
1:B:35:PRO:HB2	1:B:65:PHE:CD2	2.56	0.41
1:B:192:GLY:O	1:B:269:ARG:NH2	2.54	0.41
1:D:199:ASP:HA	1:D:200:PRO:HD3	1.91	0.41
1:A:107:THR:HG22	6:A:606:GOL:H32	2.02	0.41
1:B:259:ARG:HE	1:B:259:ARG:HB2	1.76	0.41
1:C:109:ILE:HD11	1:C:231:LEU:HD22	2.02	0.41
1:C:222:GLU:H	1:C:222:GLU:HG2	1.62	0.41
1:C:437:SER:HB3	2:C:601:HEM:HBA1	2.03	0.41
1:D:182:VAL:HG11	1:D:310:THR:HB	2.03	0.41
1:D:78:VAL:HG11	1:D:396:ILE:HD12	2.03	0.41
1:A:382:ILE:HG12	1:A:389:ILE:HB	2.02	0.40
1:B:120:PHE:CE2	3:B:602:QDN:H11	2.56	0.40
1:D:62:ARG:HE	1:D:82:ASN:HB3	1.86	0.40
1:D:379:SER:O	1:D:391:LYS:HG3	2.21	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	443/479 (92%)	430 (97%)	11 (2%)	2 (0%)	24	24
1	B	449/479 (94%)	436 (97%)	13 (3%)	0	100	100
1	C	448/479 (94%)	433 (97%)	14 (3%)	1 (0%)	43	50
1	D	444/479 (93%)	429 (97%)	15 (3%)	0	100	100
All	All	1784/1916 (93%)	1728 (97%)	53 (3%)	3 (0%)	43	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	SER
1	C	482	ALA
1	A	482	ALA

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	383/409 (94%)	375 (98%)	8 (2%)	47	58
1	B	387/409 (95%)	380 (98%)	7 (2%)	51	63
1	C	385/409 (94%)	378 (98%)	7 (2%)	51	63
1	D	385/409 (94%)	380 (99%)	5 (1%)	61	72
All	All	1540/1636 (94%)	1513 (98%)	27 (2%)	51	63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	206	LEU
1	A	213	LEU
1	A	217	SER
1	A	227	VAL
1	A	240	VAL
1	A	389	ILE
1	A	411	LYS
1	B	59	ASP
1	B	78	VAL
1	B	201	ARG
1	B	259	ARG
1	B	266	GLN
1	B	382	ILE
1	B	480	VAL
1	C	146	LYS
1	C	189	LEU
1	C	201	ARG
1	C	213	LEU
1	C	222	GLU
1	C	240	VAL
1	C	488	SER
1	D	196	GLU
1	D	414	ARG
1	D	476	SER
1	D	480	VAL
1	D	484	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	333	GLN
1	B	167	HIS
1	B	341	GLN
1	B	350	GLN
1	B	463	HIS
1	C	53	ASN
1	C	94	HIS
1	C	167	HIS
1	C	333	GLN
1	D	108	GLN
1	D	167	HIS

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Mol	Chain	Res	Type
1	D	341	GLN
1	D	350	GLN
1	D	361	HIS
1	D	424	GLN
1	D	478	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 5 are monoatomic - leaving 22 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	1	50,50,50	1.57	6 (12%)	67,82,82	1.40	10 (14%)
6	GOL	A	606	-	5,5,5	0.33	0	5,5,5	0.33	0
6	GOL	A	609	-	5,5,5	0.42	0	5,5,5	0.69	0
6	GOL	D	606	-	5,5,5	0.37	0	5,5,5	0.47	0
4	DMS	B	603	-	3,3,3	0.74	0	3,3,3	0.94	0
6	GOL	B	605	-	5,5,5	0.41	0	5,5,5	0.51	0
3	QDN	B	602	-	27,27,27	0.17	0	39,39,39	0.30	0
4	DMS	C	603	-	3,3,3	0.62	0	3,3,3	0.90	0
6	GOL	A	607	-	5,5,5	0.44	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	C	606	-	5,5,5	0.36	0	5,5,5	0.43	0
3	QDN	D	602	-	27,27,27	0.18	0	39,39,39	0.29	0
2	HEM	A	601	1	50,50,50	1.71	6 (12%)	67,82,82	1.51	13 (19%)
6	GOL	D	607	-	5,5,5	0.37	0	5,5,5	0.34	0
2	HEM	C	601	1	50,50,50	1.59	6 (12%)	67,82,82	1.26	7 (10%)
4	DMS	A	603	-	3,3,3	0.67	0	3,3,3	0.68	0
4	DMS	D	603	-	3,3,3	0.72	0	3,3,3	0.90	0
3	QDN	A	602	-	27,27,27	0.18	0	39,39,39	0.34	0
2	HEM	D	601	1	50,50,50	1.61	6 (12%)	67,82,82	1.38	9 (13%)
6	GOL	A	608	-	5,5,5	0.36	0	5,5,5	0.34	0
6	GOL	D	605	-	5,5,5	0.46	0	5,5,5	0.44	0
6	GOL	C	605	-	5,5,5	0.51	0	5,5,5	0.62	0
3	QDN	C	602	-	27,27,27	0.17	0	39,39,39	0.37	0

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	A	601	1	-	4/14/54/54	-
6	GOL	D	607	-	-	2/4/4/4	-
2	HEM	B	601	1	-	3/14/54/54	-
6	GOL	A	606	-	-	2/4/4/4	-
2	HEM	C	601	1	-	4/14/54/54	-
3	QDN	B	602	-	-	2/12/33/33	0/5/4/4
6	GOL	A	607	-	-	4/4/4/4	-
6	GOL	C	606	-	-	2/4/4/4	-
3	QDN	A	602	-	-	0/12/33/33	0/5/4/4
2	HEM	D	601	1	-	2/14/54/54	-
6	GOL	A	608	-	-	2/4/4/4	-
6	GOL	A	609	-	-	3/4/4/4	-
6	GOL	D	606	-	-	2/4/4/4	-
6	GOL	D	605	-	-	2/4/4/4	-
6	GOL	C	605	-	-	2/4/4/4	-
6	GOL	B	605	-	-	3/4/4/4	-
3	QDN	C	602	-	-	0/12/33/33	0/5/4/4
3	QDN	D	602	-	-	1/12/33/33	0/5/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	6.39	2.14	1.94
2	C	601	HEM	FE-ND	5.96	2.13	1.94
2	D	601	HEM	FE-ND	5.23	2.11	1.94
2	D	601	HEM	FE-NC	4.95	2.11	1.95
2	B	601	HEM	FE-ND	4.92	2.10	1.94
2	B	601	HEM	FE-NA	4.81	2.11	1.95
2	A	601	HEM	FE-ND	4.75	2.09	1.94
2	A	601	HEM	FE-NA	4.55	2.10	1.95
2	D	601	HEM	FE-NA	4.48	2.10	1.95
2	C	601	HEM	FE-NA	4.03	2.08	1.95
2	B	601	HEM	FE-NB	3.99	2.07	1.94
2	C	601	HEM	FE-NC	3.21	2.05	1.95
2	B	601	HEM	FE-NC	3.20	2.05	1.95
2	D	601	HEM	CAB-C3B	3.19	1.55	1.47
2	D	601	HEM	CAC-C3C	3.14	1.55	1.47
2	A	601	HEM	CAC-C3C	3.12	1.55	1.47
2	B	601	HEM	CAB-C3B	3.11	1.55	1.47
2	B	601	HEM	CAC-C3C	2.95	1.55	1.47
2	A	601	HEM	CAB-C3B	2.94	1.55	1.47
2	A	601	HEM	FE-NC	2.91	2.04	1.95
2	C	601	HEM	CAB-C3B	2.80	1.54	1.47
2	C	601	HEM	CAC-C3C	2.75	1.54	1.47
2	C	601	HEM	FE-NB	2.67	2.03	1.94
2	D	601	HEM	FE-NB	2.67	2.03	1.94

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C1B-NB-C4B	3.87	109.79	105.21
2	B	601	HEM	C4D-ND-C1D	3.83	109.75	105.21
2	A	601	HEM	C4D-ND-C1D	3.79	109.69	105.21
2	D	601	HEM	C1B-NB-C4B	3.50	109.35	105.21
2	B	601	HEM	C3D-C4D-ND	-3.42	106.42	110.17
2	B	601	HEM	C1B-NB-C4B	3.28	109.09	105.21
2	D	601	HEM	C3B-C2B-C1B	3.26	108.86	106.41
2	D	601	HEM	C4D-ND-C1D	3.19	108.99	105.21
2	D	601	HEM	CAA-CBA-CGA	-3.12	105.40	113.67
2	C	601	HEM	C4D-ND-C1D	3.06	108.83	105.21
2	C	601	HEM	C1B-NB-C4B	2.99	108.74	105.21
2	A	601	HEM	CHD-C4C-NC	2.94	127.66	124.45
2	D	601	HEM	C2B-C1B-NB	-2.92	106.49	109.84
2	A	601	HEM	C2B-C1B-NB	-2.89	106.51	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CAA-CBA-CGA	-2.81	106.22	113.67
2	B	601	HEM	C2D-C1D-ND	-2.80	106.67	109.90
2	A	601	HEM	C2D-C1D-ND	-2.78	106.69	109.90
2	A	601	HEM	C3D-C4D-ND	-2.77	107.14	110.17
2	B	601	HEM	C2A-C1A-NA	-2.65	107.21	110.15
2	A	601	HEM	C3B-C2B-C1B	2.60	108.36	106.41
2	D	601	HEM	C2D-C1D-ND	-2.52	106.99	109.90
2	C	601	HEM	C3B-C2B-C1B	2.50	108.29	106.41
2	C	601	HEM	CAA-CBA-CGA	-2.45	107.17	113.67
2	C	601	HEM	C2B-C1B-NB	-2.42	107.06	109.84
2	C	601	HEM	C2A-C1A-NA	-2.42	107.47	110.15
2	D	601	HEM	C3D-C4D-ND	-2.39	107.55	110.17
2	B	601	HEM	CHC-C4B-NB	2.38	126.98	124.42
2	A	601	HEM	C2A-C1A-NA	-2.29	107.61	110.15
2	D	601	HEM	CHC-C4B-NB	2.27	126.87	124.42
2	B	601	HEM	CAA-CBA-CGA	-2.26	107.68	113.67
2	B	601	HEM	C2B-C1B-NB	-2.24	107.26	109.84
2	A	601	HEM	C4C-NC-C1C	2.24	109.47	105.82
2	D	601	HEM	C2A-C1A-NA	-2.18	107.73	110.15
2	B	601	HEM	C4A-NA-C1A	2.13	109.29	105.82
2	A	601	HEM	C3B-C4B-NB	-2.13	107.94	109.47
2	C	601	HEM	C4A-NA-C1A	2.08	109.22	105.82
2	A	601	HEM	O2D-CGD-CBD	2.07	120.53	114.00
2	A	601	HEM	CBD-CAD-C3D	-2.05	106.87	112.53
2	B	601	HEM	C3B-C2B-C1B	2.03	107.94	106.41

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	607	GOL	O1-C1-C2-C3
6	A	608	GOL	O1-C1-C2-C3
6	C	605	GOL	C1-C2-C3-O3
6	C	605	GOL	O2-C2-C3-O3
6	C	606	GOL	O1-C1-C2-C3
6	D	606	GOL	O1-C1-C2-C3
6	A	607	GOL	O1-C1-C2-O2
6	C	606	GOL	O1-C1-C2-O2
6	A	607	GOL	C1-C2-C3-O3
6	A	609	GOL	O1-C1-C2-C3
6	B	605	GOL	O1-C1-C2-C3
6	D	605	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	D	606	GOL	O1-C1-C2-O2
6	A	607	GOL	O2-C2-C3-O3
6	A	608	GOL	O1-C1-C2-O2
3	B	602	QDN	C13-C17-C18-C19
6	A	606	GOL	O1-C1-C2-O2
6	A	609	GOL	O2-C2-C3-O3
6	B	605	GOL	O1-C1-C2-O2
6	D	605	GOL	O1-C1-C2-O2
6	D	607	GOL	O1-C1-C2-O2
6	A	609	GOL	O1-C1-C2-O2
3	D	602	QDN	C13-C17-C18-C19
6	A	606	GOL	O1-C1-C2-C3
2	B	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O2A
6	B	605	GOL	O2-C2-C3-O3
2	B	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O1A
2	D	601	HEM	CAA-CBA-CGA-O1A
3	B	602	QDN	C16-C17-C18-C19
6	D	607	GOL	O1-C1-C2-C3
2	B	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	C	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

12 monomers are involved in 22 short contacts:

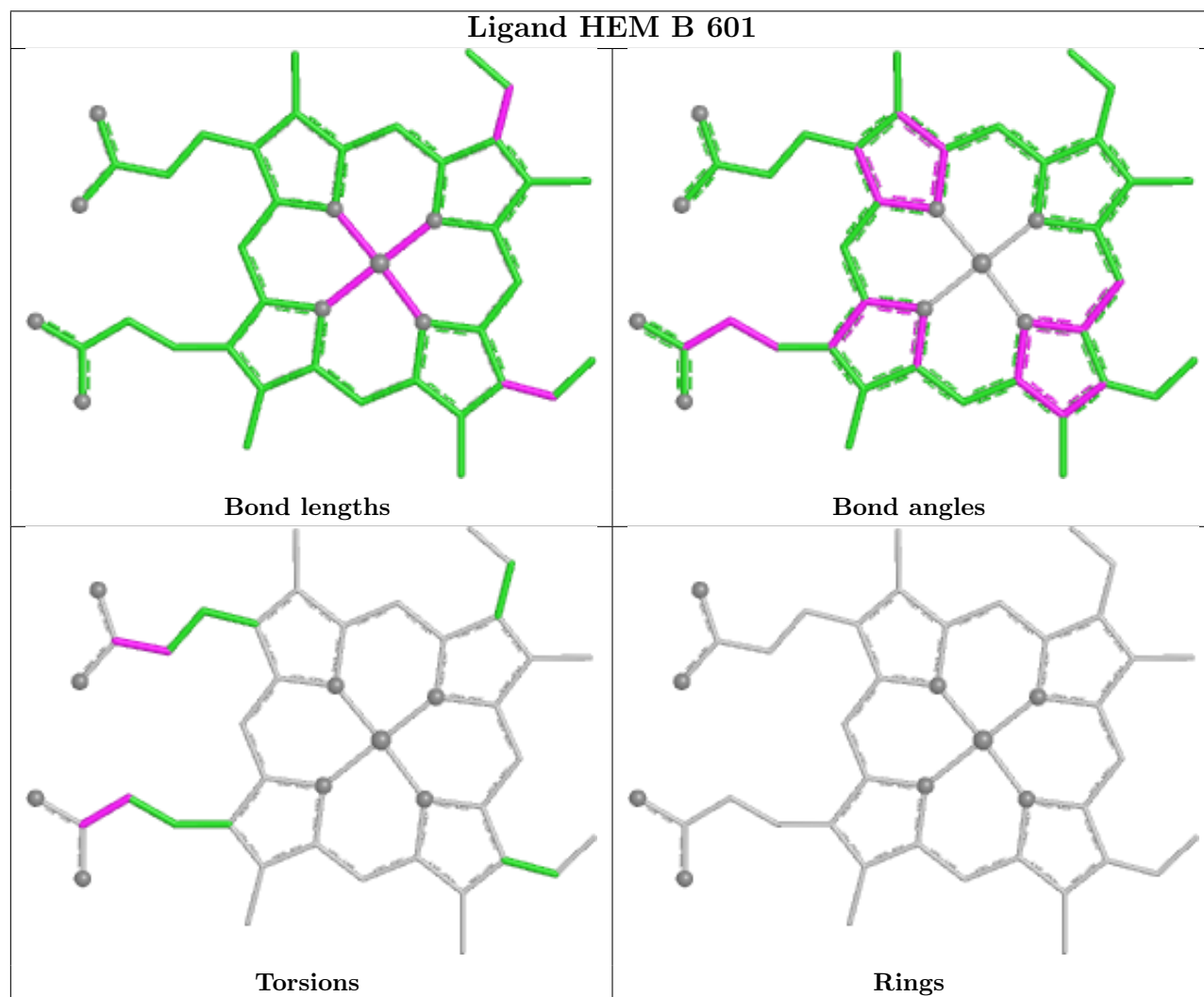
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	1	0
6	A	606	GOL	1	0
6	A	609	GOL	1	0
6	B	605	GOL	3	0
3	B	602	QDN	1	0
6	A	607	GOL	1	0
6	D	607	GOL	1	0
2	C	601	HEM	2	0
3	A	602	QDN	2	0

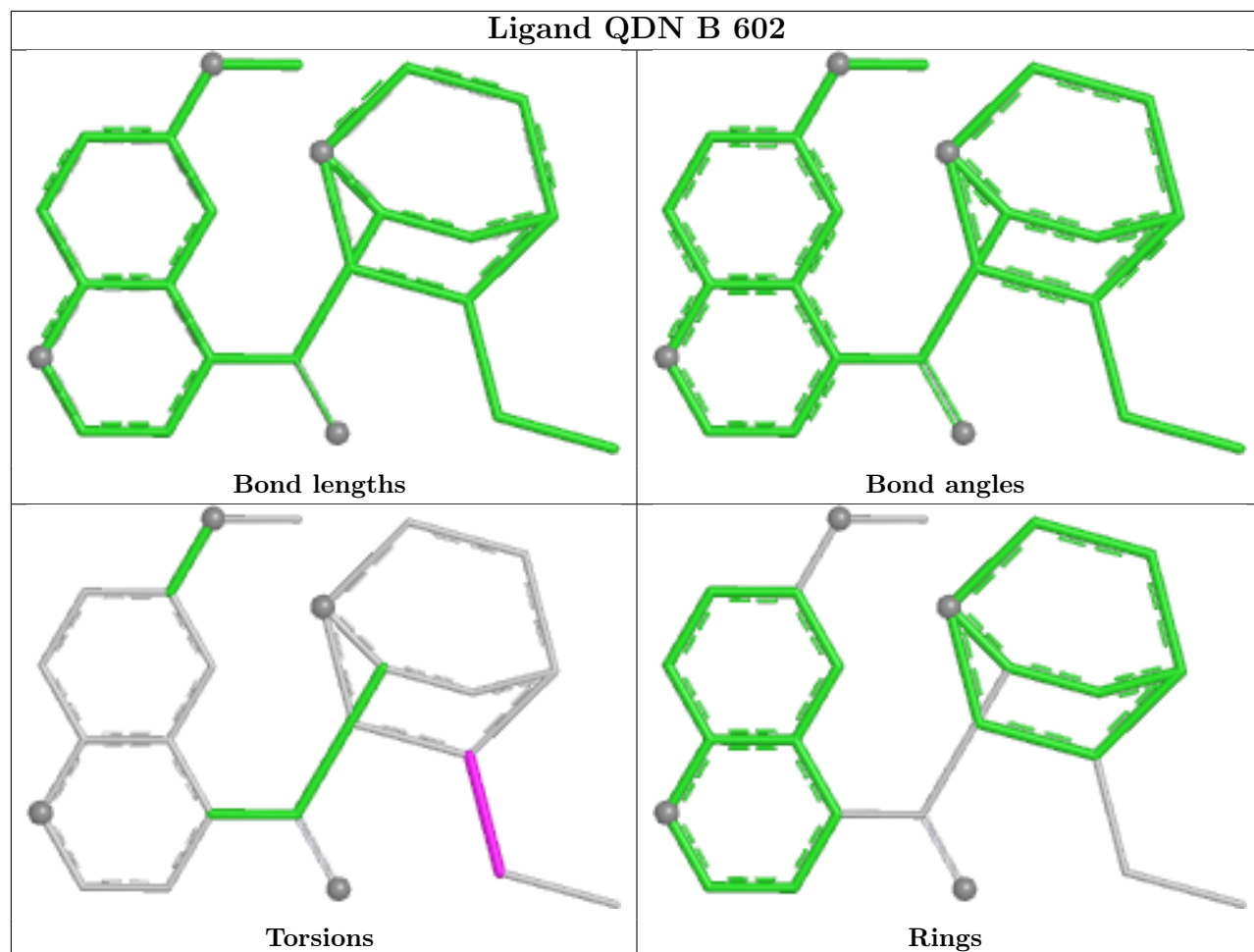
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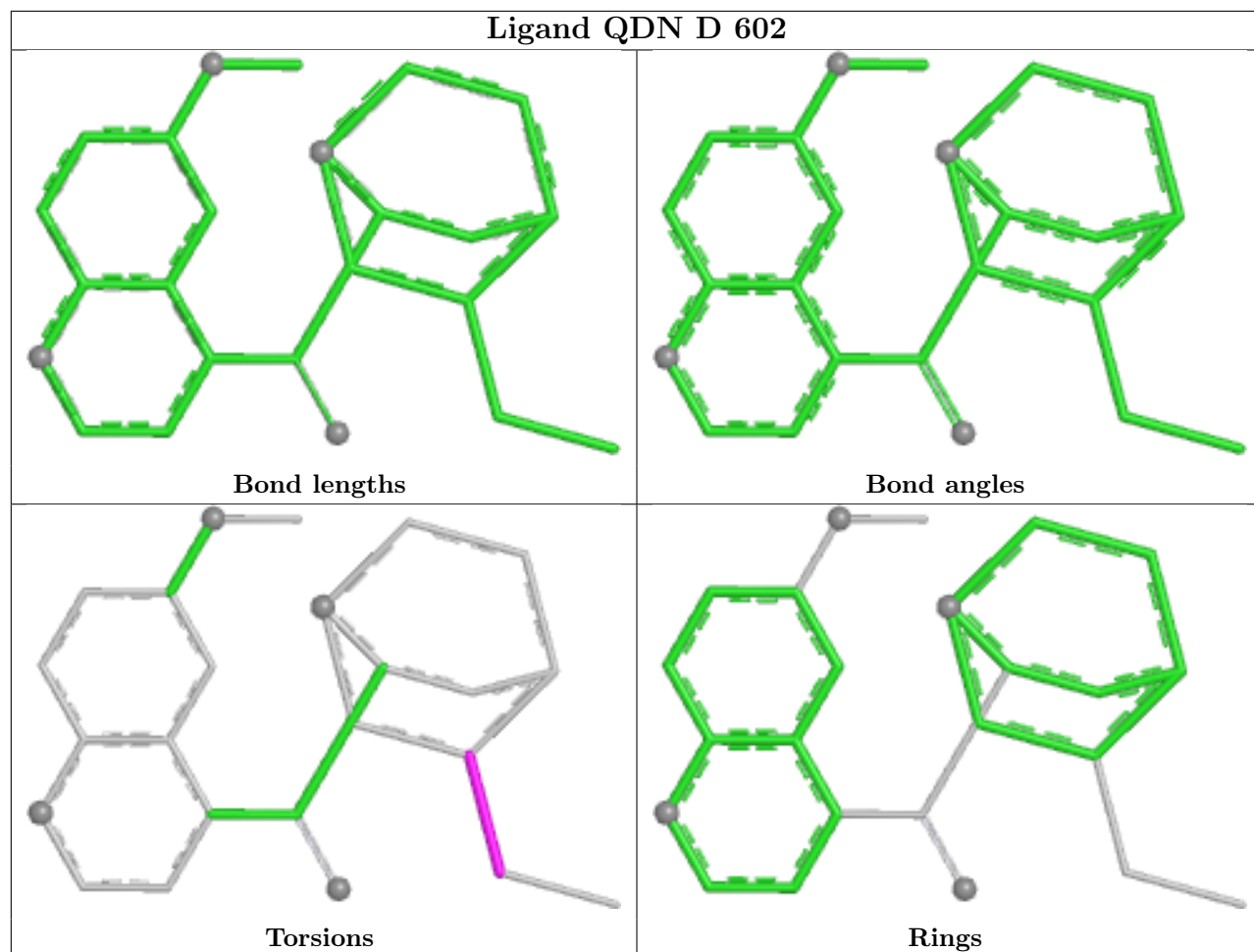
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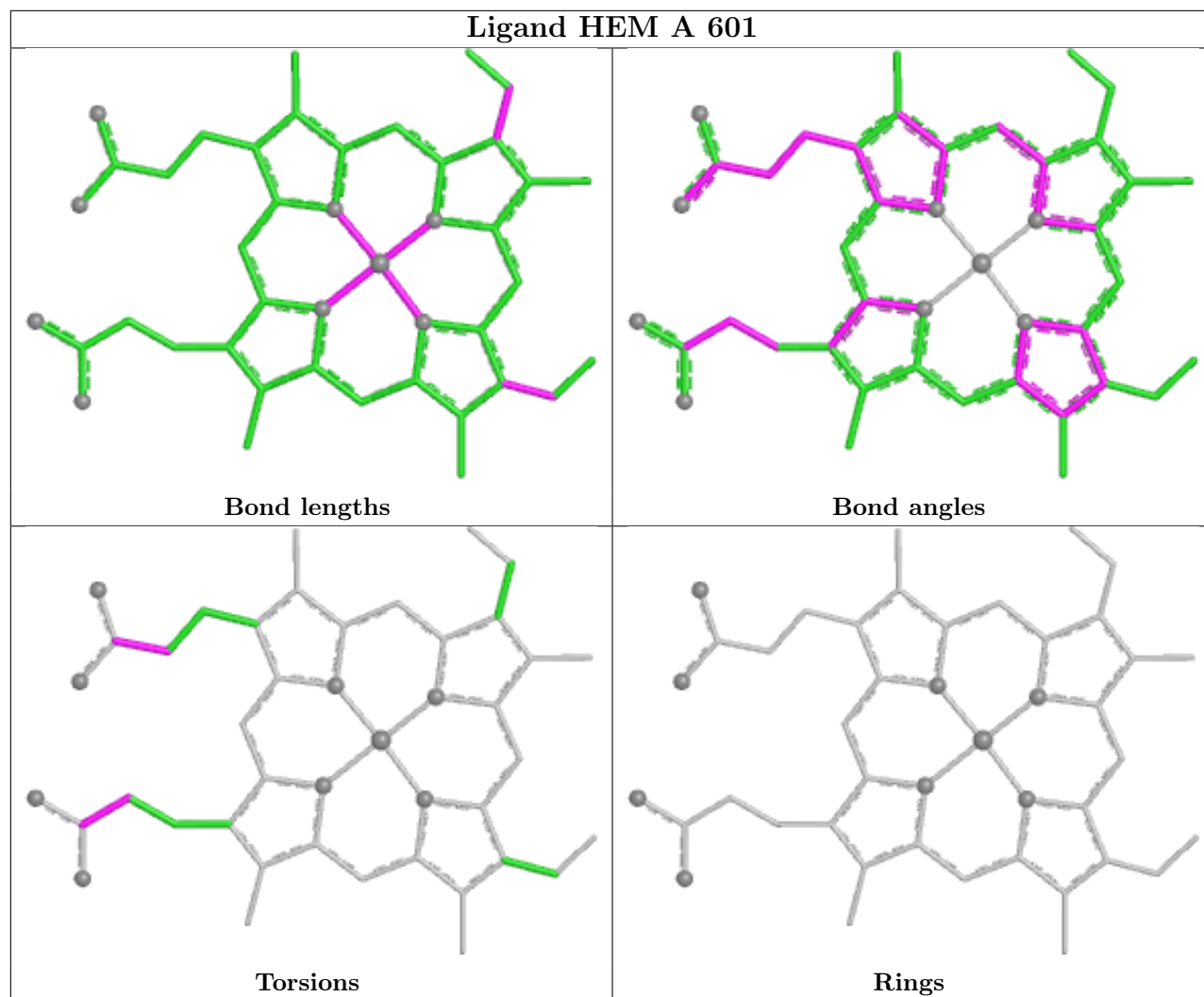
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	3	0
6	D	605	GOL	3	0
6	C	605	GOL	3	0

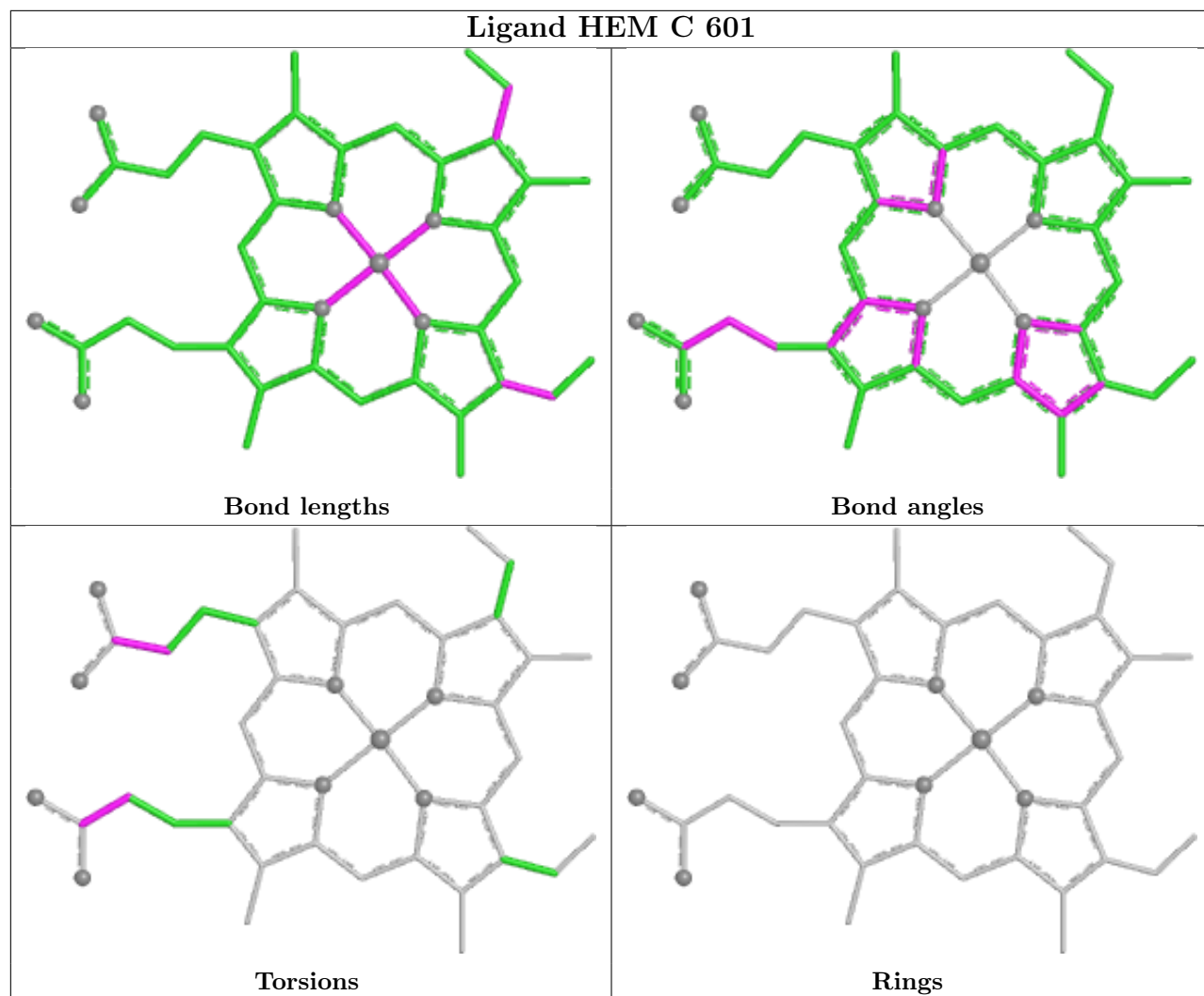
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

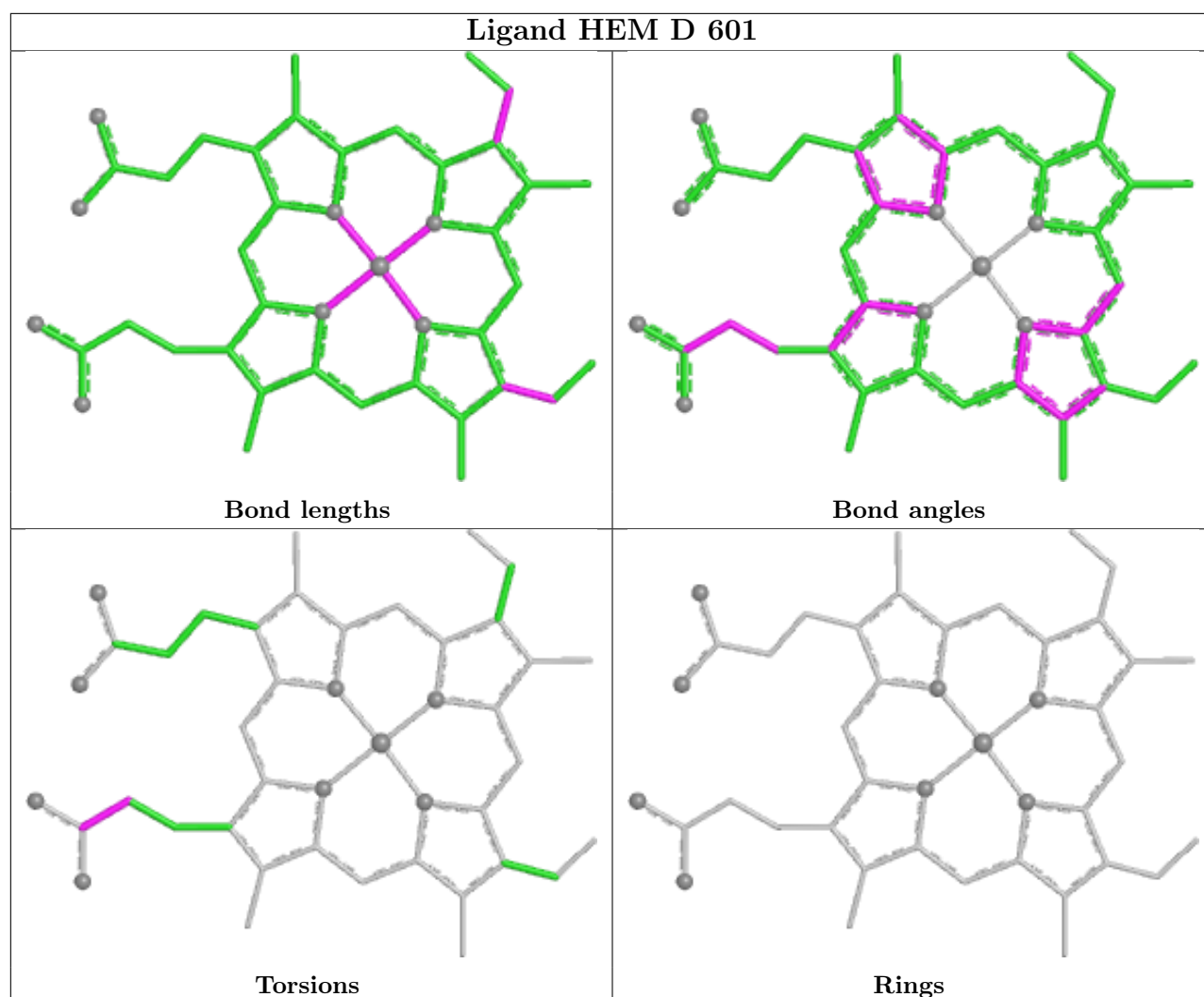












5.7 Other polymers [i](#)

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	449/479 (93%)	0.24	26 (5%)	29	27	23, 39, 78, 110	0
1	B	453/479 (94%)	0.44	39 (8%)	16	15	25, 49, 87, 108	0
1	C	452/479 (94%)	0.28	37 (8%)	17	16	23, 41, 85, 110	0
1	D	450/479 (93%)	0.55	35 (7%)	19	17	27, 53, 90, 114	0
All	All	1804/1916 (94%)	0.38	137 (7%)	20	18	23, 46, 86, 114	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	PHE	6.0
1	A	144	LEU	5.7
1	D	143	GLY	5.6
1	B	143	GLY	5.6
1	C	483	PHE	5.1
1	A	75	TRP	5.0
1	B	144	LEU	4.9
1	C	144	LEU	4.8
1	B	37	PRO	4.7
1	A	482	ALA	4.7
1	D	75	TRP	4.6
1	C	481	PHE	4.5
1	C	219	PHE	4.4
1	B	75	TRP	4.4
1	A	219	PHE	4.4
1	C	53	ASN	4.3
1	B	480	VAL	4.3
1	D	37	PRO	4.2
1	D	219	PHE	4.1
1	D	470	THR	4.1
1	A	481	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	3.8
1	A	59	ASP	3.6
1	B	219	PHE	3.6
1	C	482	ALA	3.6
1	C	240	VAL	3.6
1	B	51	PHE	3.5
1	C	146	LYS	3.4
1	B	145	GLY	3.4
1	C	380	ARG	3.4
1	B	142	LEU	3.4
1	B	470	THR	3.4
1	D	115	ARG	3.4
1	D	342	VAL	3.4
1	C	75	TRP	3.3
1	C	143	GLY	3.2
1	D	482	ALA	3.2
1	A	96	GLU	3.1
1	A	74	ALA	3.1
1	D	51	PHE	3.1
1	B	423	ALA	3.1
1	C	238	GLY	3.0
1	C	62	ARG	2.9
1	A	238	GLY	2.9
1	A	470	THR	2.9
1	B	483	PHE	2.9
1	C	220	LEU	2.9
1	D	33	LEU	2.9
1	C	227	VAL	2.9
1	A	235	ALA	2.8
1	B	170	ARG	2.8
1	D	147	LYS	2.8
1	D	229	VAL	2.8
1	C	239	LYS	2.7
1	D	65	PHE	2.7
1	B	239	LYS	2.7
1	B	33	LEU	2.7
1	B	147	LYS	2.7
1	B	52	GLN	2.6
1	C	235	ALA	2.6
1	C	74	ALA	2.6
1	C	59	ASP	2.6
1	B	342	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	238	GLY	2.6
1	B	57	CYS	2.6
1	D	96	GLU	2.6
1	B	240	VAL	2.6
1	C	223	VAL	2.6
1	C	233	ILE	2.6
1	B	479	GLY	2.5
1	C	236	LEU	2.5
1	B	74	ALA	2.5
1	D	463	HIS	2.5
1	D	483	PHE	2.5
1	B	72	GLN	2.5
1	D	116	SER	2.5
1	B	115	ARG	2.5
1	D	53	ASN	2.5
1	D	425	GLY	2.5
1	B	32	LYS	2.5
1	B	471	GLY	2.5
1	C	169	GLY	2.5
1	D	481	PHE	2.4
1	D	233	ILE	2.4
1	C	73	LEU	2.4
1	C	168	SER	2.4
1	C	342	VAL	2.4
1	D	480	VAL	2.4
1	C	237	ALA	2.4
1	D	239	LYS	2.4
1	C	63	ARG	2.4
1	A	53	ASN	2.4
1	D	234	PRO	2.4
1	B	413	PHE	2.4
1	D	63	ARG	2.4
1	A	239	LYS	2.3
1	B	63	ARG	2.3
1	B	380	ARG	2.3
1	D	236	LEU	2.3
1	C	234	PRO	2.3
1	A	240	VAL	2.3
1	C	61	LEU	2.3
1	A	56	TYR	2.3
1	A	380	ARG	2.3
1	A	70	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	218	GLY	2.2
1	D	423	ALA	2.2
1	B	472	GLN	2.2
1	B	481	PHE	2.2
1	D	169	GLY	2.2
1	B	96	GLU	2.2
1	B	482	ALA	2.2
1	D	73	LEU	2.2
1	A	37	PRO	2.2
1	B	169	GLY	2.2
1	C	217	SER	2.2
1	C	56	TYR	2.2
1	C	96	GLU	2.2
1	D	424	GLN	2.2
1	D	56	TYR	2.1
1	A	61	LEU	2.1
1	C	145	GLY	2.1
1	D	170	ARG	2.1
1	A	342	VAL	2.1
1	B	235	ALA	2.1
1	D	469	PRO	2.1
1	B	65	PHE	2.1
1	A	62	ARG	2.1
1	B	341	GLN	2.0
1	A	225	ASN	2.0
1	D	109	ILE	2.0
1	D	235	ALA	2.0
1	A	333	GLN	2.0
1	A	484	LEU	2.0
1	C	230	LEU	2.0
1	C	37	PRO	2.0
1	C	388	ARG	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 ⓘ

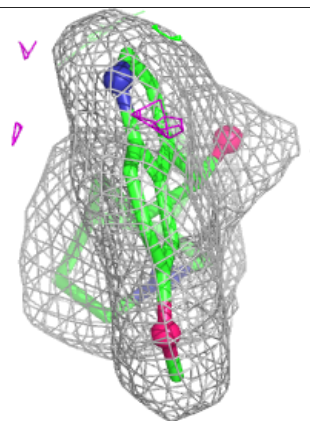
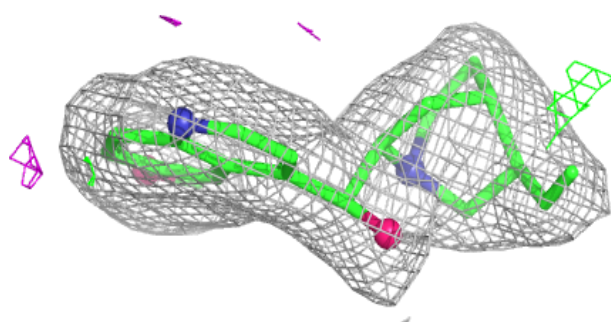
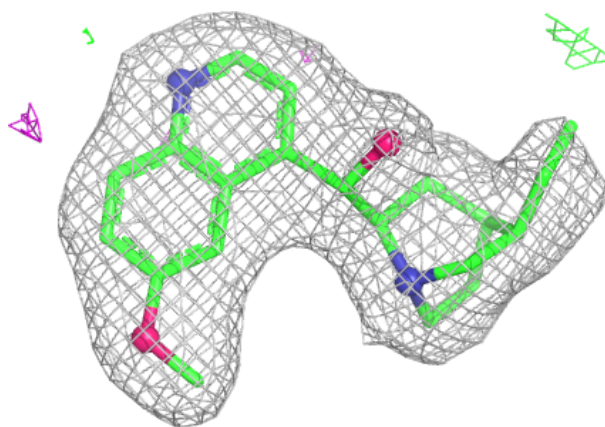
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	D	606	6/6	0.79	0.25	99,100,102,102	0
6	GOL	C	606	6/6	0.81	0.24	93,94,96,96	0
6	GOL	A	609	6/6	0.82	0.20	47,52,53,55	0
6	GOL	A	607	6/6	0.83	0.19	62,65,66,67	0
6	GOL	D	607	6/6	0.83	0.16	84,86,88,89	0
4	DMS	B	603	4/4	0.85	0.18	46,53,82,83	0
6	GOL	A	608	6/6	0.86	0.17	86,88,88,89	0
4	DMS	A	603	4/4	0.89	0.17	49,67,76,77	0
4	DMS	D	603	4/4	0.90	0.15	50,54,71,72	0
6	GOL	D	605	6/6	0.91	0.12	56,59,59,60	0
4	DMS	C	603	4/4	0.92	0.13	34,45,68,70	0
6	GOL	B	605	6/6	0.94	0.10	46,51,51,53	0
6	GOL	C	605	6/6	0.94	0.09	48,49,49,49	0
3	QDN	C	602	24/24	0.95	0.08	36,39,41,46	0
3	QDN	D	602	24/24	0.95	0.09	37,41,44,45	0
3	QDN	B	602	24/24	0.95	0.08	33,36,39,46	0
6	GOL	A	606	6/6	0.96	0.11	37,43,43,45	0
3	QDN	A	602	24/24	0.96	0.08	36,38,42,48	0
2	HEM	C	601	43/43	0.98	0.05	19,23,30,39	0
2	HEM	D	601	43/43	0.98	0.06	22,30,33,35	0
2	HEM	A	601	43/43	0.98	0.05	17,23,26,28	0
2	HEM	B	601	43/43	0.98	0.06	22,28,32,36	0
5	ZN	B	604	1/1	0.99	0.03	34,34,34,34	0
5	ZN	D	604	1/1	0.99	0.02	38,38,38,38	0
5	ZN	C	604	1/1	1.00	0.03	36,36,36,36	0
5	ZN	A	605	1/1	1.00	0.01	42,42,42,42	0
5	ZN	A	604	1/1	1.00	0.02	32,32,32,32	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.

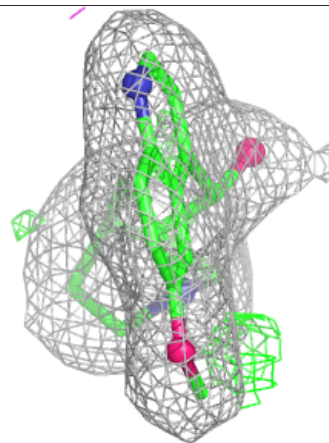
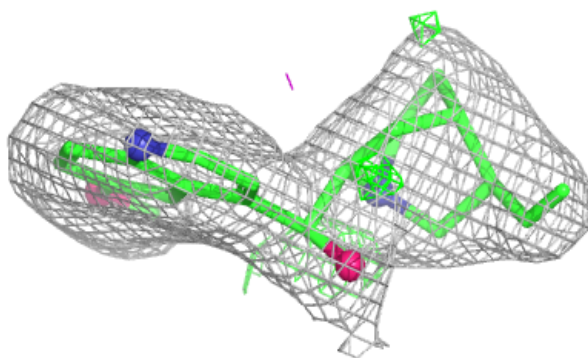
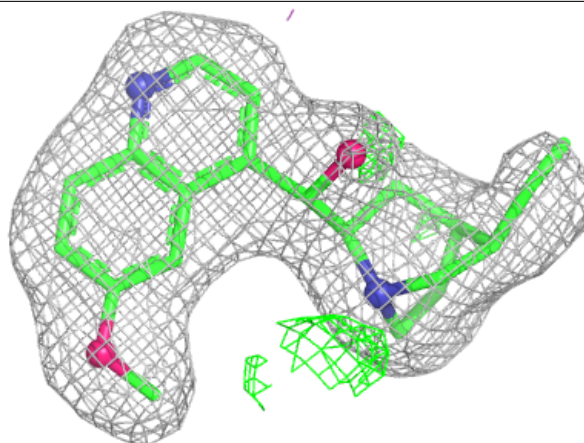
Electron density around QDN D 602:

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



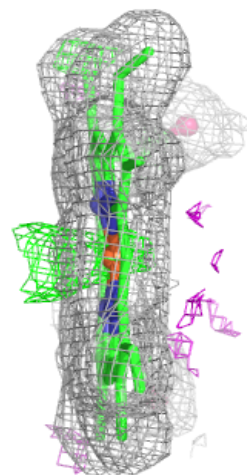
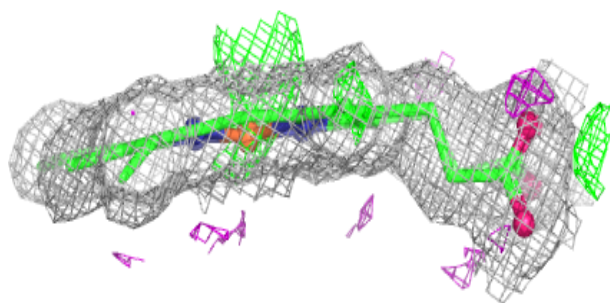
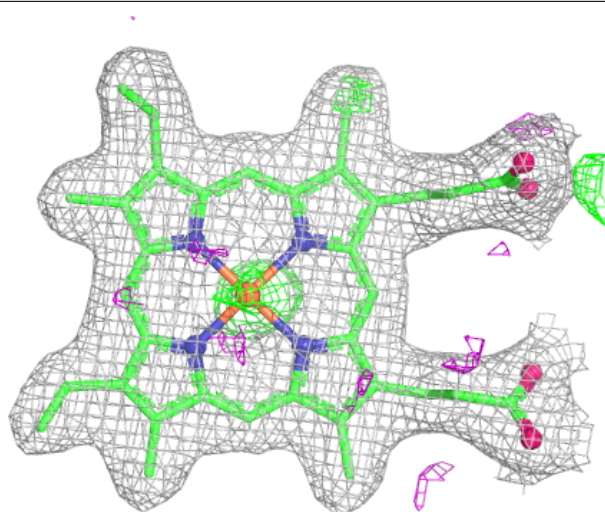
Electron density around QDN B 602:

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



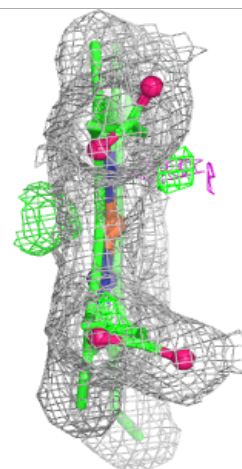
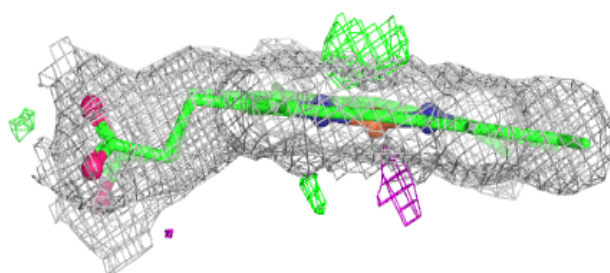
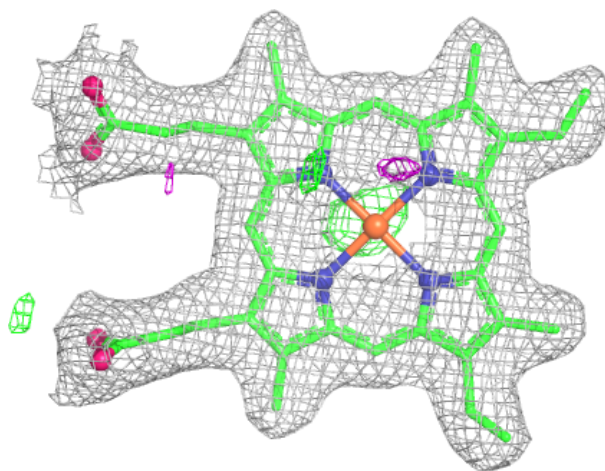
Electron density around HEM C 601:

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



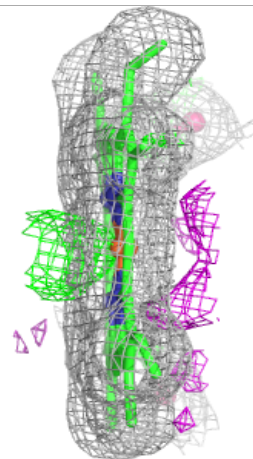
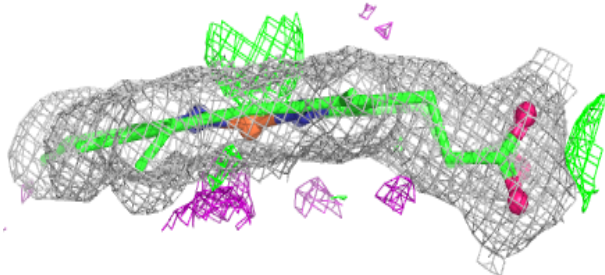
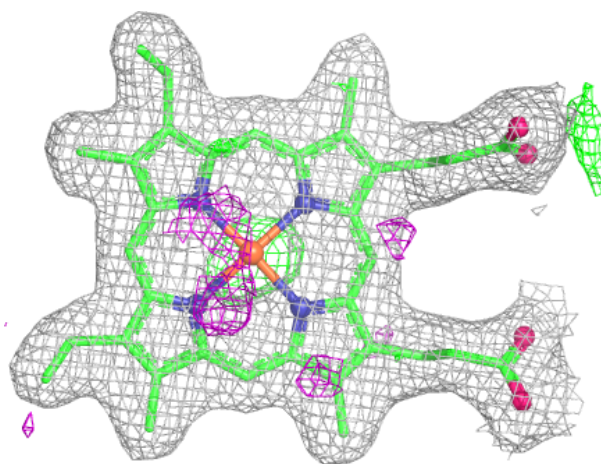
Electron density around HEM D 601:

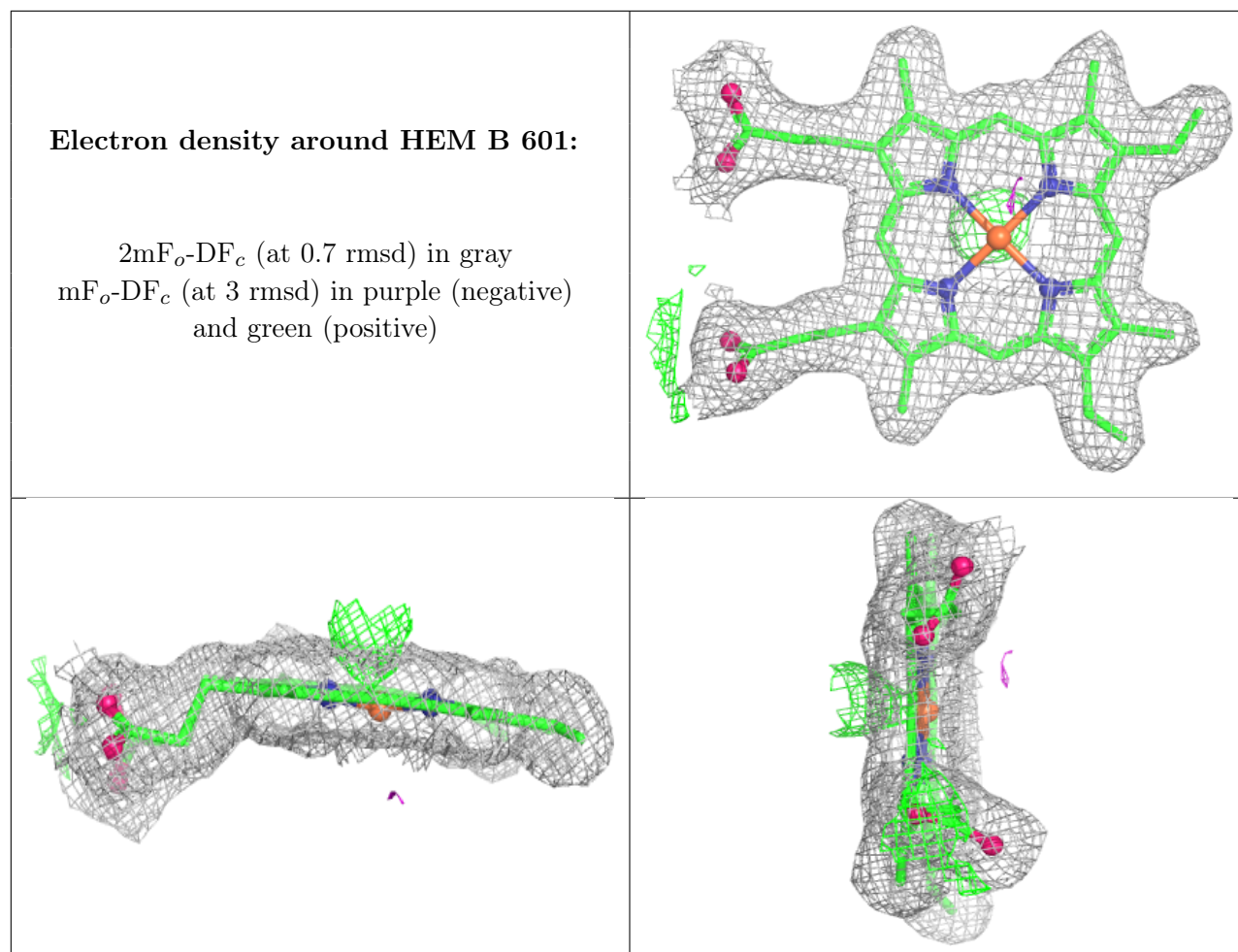
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.