



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:25 PM UTC

PDB ID : 5TE8 / pdb_00005te8
Title : Crystal structure of the midazolam-bound human CYP3A4
Authors : Sevrioukova, I.; Poulos, T.
Deposited on : 2016-09-20
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 : 4-5-2 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

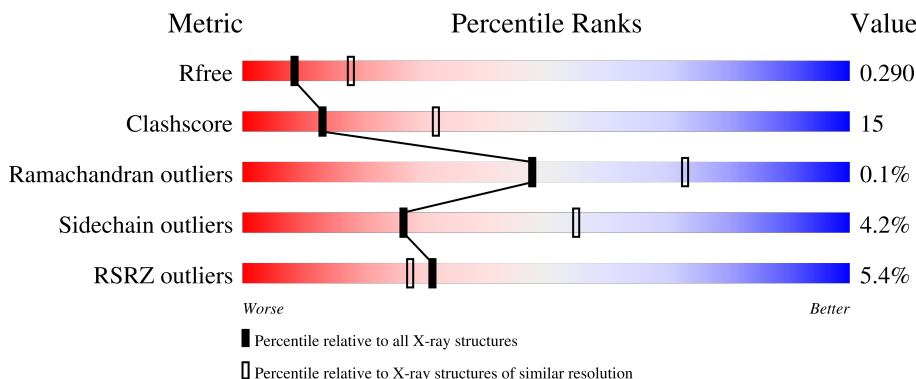
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	487	2% 69% 26% ..
1	B	487	3% 72% 23% ..
1	C	487	10% 58% 35% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	08J	A	602	-	-	X	-
3	08J	C	602	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11681 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 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	1	0
			3796	2470	626	676	24			
1	B	471	Total	C	N	O	S	0	0	0
			3797	2469	626	678	24			
1	C	469	Total	C	N	O	S	0	0	0
			3779	2459	622	674	24			

There are 18 discrepancies between the modelled and reference sequences:

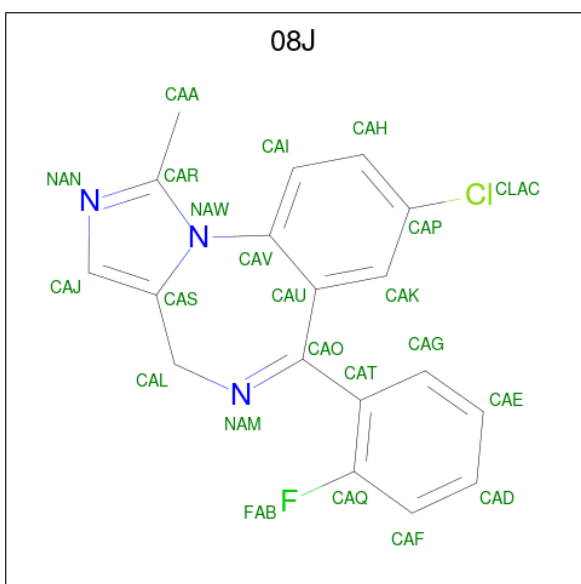
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	see remark 999	UNP P08684
A	2	ALA	-	see remark 999	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	1	MET	-	see remark 999	UNP P08684
B	2	ALA	-	see remark 999	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684
C	1	MET	-	see remark 999	UNP P08684
C	2	ALA	-	see remark 999	UNP P08684
C	504	HIS	-	expression tag	UNP P08684
C	505	HIS	-	expression tag	UNP P08684
C	506	HIS	-	expression tag	UNP P08684
C	507	HIS	-	expression tag	UNP P08684

- 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

- Molecule 3 is 8-chloro-6-(2-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepine (CCD ID: 08J) (formula: C₁₈H₁₃ClFN₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	0	0
			23	18	1	1	3		
3	B	1	Total	C	Cl	F	N	0	0
			23	18	1	1	3		
3	C	1	Total	C	Cl	F	N	0	0
			23	18	1	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	42	Total	O	0	0
			42	42		
4	C	16	Total	O	0	0
			16	16		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.29Å 117.98Å 205.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.34 – 2.70 102.34 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (102.34-2.70) 98.8 (102.34-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.224 , 0.292 0.235 , 0.290	Depositor DCC
R_{free} test set	2178 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11681	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 08J

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	0.49	0/3889	0.96	11/5260 (0.2%)
1	B	0.49	0/3891	0.96	7/5264 (0.1%)
1	C	0.50	0/3872	0.93	6/5238 (0.1%)
All	All	0.50	0/11652	0.95	24/15762 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	GLU	N-CA-C	-10.87	100.14	113.41
1	B	259	SER	N-CA-C	10.48	128.56	111.37
1	A	265	GLN	N-CA-C	9.95	124.07	111.24
1	B	307	TYR	N-CA-C	9.71	121.55	110.97
1	B	225	VAL	N-CA-C	-9.66	99.29	110.21
1	C	334	GLU	N-CA-C	-8.43	102.98	113.18
1	A	243	ARG	CB-CA-C	-7.71	95.07	110.42
1	B	260	ARG	N-CA-C	-7.34	104.32	113.28
1	B	438	GLY	CA-C-N	6.70	126.40	119.56
1	B	438	GLY	C-N-CA	6.70	126.40	119.56
1	A	265	GLN	CB-CA-C	-6.58	100.01	110.86
1	C	163	GLU	N-CA-CB	6.44	123.11	113.65
1	A	324	HIS	CA-C-N	6.15	126.04	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	HIS	C-N-CA	6.15	126.04	119.28
1	A	108	PHE	N-CA-C	6.14	121.16	113.43
1	C	418	ARG	N-CA-C	-6.12	105.68	113.02
1	C	341	ASN	N-CA-C	-5.72	94.97	111.00
1	B	259	SER	CB-CA-C	-5.42	101.84	110.84
1	C	241	PHE	CA-C-N	5.41	125.35	119.78
1	C	241	PHE	C-N-CA	5.41	125.35	119.78
1	A	266	LYS	N-CA-C	-5.38	101.50	110.17
1	A	269	VAL	N-CA-C	5.35	116.67	111.91
1	A	241	PHE	CA-C-N	5.10	124.41	118.85
1	A	241	PHE	C-N-CA	5.10	124.41	118.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	333	GLU	Peptide
1	C	418	ARG	Sidechain

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	3796	0	3876	105	0
1	B	3797	0	3873	84	0
1	C	3779	0	3862	146	1
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	6	0
3	A	23	0	13	7	0
3	B	23	0	13	1	0
3	C	23	0	13	12	0
4	A	53	0	0	7	0
4	B	42	0	0	2	0
4	C	16	0	0	2	0
All	All	11681	0	11740	347	1

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 15.

All (347) 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:369:ILE:HD11	3:C:602:08J:CLAC	1.32	1.59
1:C:369:ILE:CD1	3:C:602:08J:CLAC	2.03	1.41
3:C:602:08J:H4	3:C:602:08J:H3	1.40	1.00
1:C:362:GLU:HG3	1:C:418:ARG:NH2	1.83	0.93
1:C:369:ILE:HD13	3:C:602:08J:CLAC	2.07	0.91
1:C:309:THR:HG21	3:C:602:08J:CLAC	2.10	0.88
1:A:242:PRO:O	1:A:243:ARG:HB2	1.72	0.87
1:A:260:ARG:O	1:A:263:ASP:O	1.92	0.87
1:C:413:LYS:HG3	1:C:418:ARG:NH1	1.90	0.86
1:A:111:VAL:HG12	1:A:114:MET:HB2	1.58	0.84
1:C:339:LEU:HB3	1:C:343:ALA:HB3	1.60	0.84
1:C:254:LYS:O	1:C:258:GLU:HB2	1.79	0.82
3:C:602:08J:H4	3:C:602:08J:CAI	2.10	0.82
1:B:252:SER:O	1:B:256:MET:HB2	1.79	0.81
1:C:257:LYS:HA	1:C:260:ARG:HG3	1.62	0.81
1:C:331:LEU:HG	1:C:334:GLU:HB3	1.63	0.79
1:B:287:HIS:CD2	1:B:288:LYS:HD2	2.19	0.76
1:C:424:LYS:HB3	1:C:427:ILE:HD13	1.66	0.76
1:C:329:GLN:HA	1:C:332:GLN:HB2	1.66	0.76
1:C:373:LEU:HB2	1:C:396:ILE:HB	1.68	0.75
1:B:287:HIS:HD2	1:B:288:LYS:HD2	1.52	0.74
1:C:87:PRO:HG3	1:C:431:ILE:HD11	1.70	0.74
1:C:261:LEU:HD12	1:C:268:ARG:HH11	1.52	0.74
1:B:338:VAL:HG21	1:B:352:GLN:HG2	1.69	0.73
1:B:300:ILE:HA	1:B:303:ILE:HD12	1.71	0.72
1:C:362:GLU:HG2	1:C:416:PRO:HA	1.71	0.72
1:B:478:SER:OG	1:B:484:GLN:HB3	1.89	0.72
2:C:601:HEM:HMD1	2:C:601:HEM:HBD2	1.72	0.72
1:C:379:LYS:HA	1:C:390:LYS:HB2	1.71	0.72
1:A:71:VAL:HG21	1:A:386:MET:HE1	1.71	0.72
1:C:110:PRO:HG3	1:C:234:GLU:HG3	1.70	0.71
1:A:141:LYS:HD2	1:A:274:LEU:HD22	1.71	0.71
2:C:601:HEM:HBB2	2:C:601:HEM:HMB2	1.71	0.71
1:B:371:MET:O	1:B:371:MET:HG2	1.91	0.70
1:A:210:LEU:HD21	1:A:300:ILE:HG23	1.74	0.69
1:B:76:ASP:OD2	1:B:106:ARG:NH2	2.25	0.69
1:B:160:LEU:HD13	1:B:175:VAL:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HA	1:A:66:LYS:HE3	1.74	0.69
1:C:418:ARG:NH2	4:C:701:HOH:O	2.20	0.69
1:B:237:ASN:HB3	4:B:719:HOH:O	1.93	0.69
1:B:157:VAL:HG23	1:B:463:PHE:CE2	2.28	0.68
1:C:415:LEU:H	1:C:418:ARG:HH12	1.42	0.67
1:C:419:PHE:C	1:C:424:LYS:HG3	2.20	0.67
1:C:111:VAL:HG21	1:C:215:PHE:CZ	2.31	0.66
1:C:99:TYR:HD1	1:C:127:LYS:HE2	1.60	0.65
1:C:369:ILE:HD11	3:C:602:08J:CAP	2.26	0.65
2:C:601:HEM:HMD1	2:C:601:HEM:CBD	2.27	0.65
1:A:370:ALA:O	1:A:371:MET:HB2	1.96	0.64
1:C:152:TYR:OH	1:C:192:ASN:HA	1.98	0.64
1:A:55:LYS:HB3	1:A:59:MET:HB2	1.79	0.64
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.80	0.64
1:B:152:TYR:CD1	1:B:182:ASP:HB3	2.34	0.63
1:C:413:LYS:HG3	1:C:418:ARG:HH12	1.62	0.63
1:A:141:LYS:HD2	1:A:274:LEU:CD2	2.28	0.63
1:B:128:ARG:NH2	1:B:289:ALA:O	2.32	0.62
1:C:179:TYR:CZ	1:C:455:ALA:HB2	2.35	0.62
1:C:23:TYR:OH	1:C:32:LEU:HD21	1.99	0.62
1:C:336:ASP:O	1:C:340:PRO:HB3	1.99	0.62
1:C:226:PHE:CE1	1:C:228:PHE:HB2	2.34	0.62
1:C:290:LEU:HD23	1:C:291:SER:O	1.99	0.62
1:C:336:ASP:OD2	1:C:341:ASN:HB2	1.98	0.62
1:A:242:PRO:O	1:A:243:ARG:CB	2.44	0.62
1:A:118:ILE:H	1:A:298:GLN:HE22	1.47	0.61
1:B:369:ILE:HA	1:B:483:LEU:HB2	1.83	0.61
1:C:143:LYS:O	1:C:146:VAL:HG22	2.01	0.61
1:B:324:HIS:NE2	1:B:413:LYS:NZ	2.48	0.60
1:A:87:PRO:HG3	1:A:431:ILE:HD11	1.83	0.60
1:C:128:ARG:O	1:C:132:LEU:HG	2.02	0.60
1:C:290:LEU:HG	1:C:294:GLU:HB3	1.84	0.60
1:A:269:VAL:HG22	1:A:269:VAL:O	2.02	0.60
1:B:340:PRO:O	1:B:341:ASN:HB2	2.01	0.60
1:A:106:ARG:HD2	1:A:374:GLU:OE1	2.03	0.59
1:C:186:SER:HA	1:C:191:VAL:H	1.66	0.59
1:A:264:THR:HG22	1:A:264:THR:O	2.03	0.58
1:B:156:LEU:HD13	1:B:179:TYR:HB2	1.84	0.58
1:C:317:ILE:HG21	1:C:456:LEU:HD11	1.84	0.58
1:A:63:GLU:HG2	1:A:66:LYS:HE3	1.85	0.58
1:B:47:LEU:O	1:B:50:ILE:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ARG:O	1:A:497:ASP:HB2	2.03	0.58
1:A:371:MET:HE1	1:A:481:GLY:C	2.29	0.58
1:C:221:LEU:HD21	1:C:240:VAL:HG11	1.85	0.58
1:C:363:THR:O	1:C:367:PHE:N	2.34	0.58
1:A:317:ILE:HD13	1:A:456:LEU:HD11	1.85	0.57
1:C:71:VAL:HG11	1:C:386:MET:HE1	1.84	0.57
1:C:309:THR:CG2	3:C:602:08J:CLAC	2.88	0.57
1:B:328:GLN:O	1:B:332:GLN:HB2	2.05	0.57
1:B:87:PRO:HG3	1:B:431:ILE:HD11	1.85	0.57
1:C:341:ASN:O	1:C:342:LYS:HB2	2.05	0.56
1:C:413:LYS:CG	1:C:418:ARG:NH1	2.67	0.56
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.88	0.56
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.86	0.56
1:A:253:VAL:O	1:A:257:LYS:HG2	2.06	0.56
1:B:338:VAL:C	1:B:340:PRO:HD3	2.30	0.56
2:A:601:HEM:HAA1	3:A:602:08J:H8	1.88	0.55
1:A:257:LYS:N	4:A:701:HOH:O	2.39	0.55
1:A:415:LEU:O	1:A:418:ARG:HG3	2.06	0.55
1:A:180:SER:O	1:A:184[A]:ILE:HG13	2.07	0.55
1:B:288:LYS:O	1:B:289:ALA:HB3	2.06	0.55
1:C:146:VAL:HG21	1:C:347:TYR:HB2	1.89	0.55
1:A:305:ALA:HB2	3:A:602:08J:CAA	2.37	0.55
3:C:602:08J:CAI	3:C:602:08J:CAA	2.79	0.55
1:A:57:PHE:HD1	1:A:57:PHE:H	1.53	0.54
1:A:371:MET:CE	1:A:481:GLY:C	2.80	0.54
1:C:335:ILE:HD11	1:C:457:ILE:HA	1.89	0.54
1:A:243:ARG:O	1:A:243:ARG:HG3	2.07	0.54
1:C:292:ASP:O	1:C:295:LEU:HB3	2.07	0.54
2:A:601:HEM:HMC1	2:A:601:HEM:HBC2	1.89	0.54
1:C:260:ARG:HG2	1:C:261:LEU:H	1.73	0.54
1:A:148:ILE:HD12	1:A:148:ILE:N	2.23	0.54
1:A:189:PHE:CE2	1:A:303:ILE:HD11	2.43	0.53
1:A:257:LYS:HG3	4:A:701:HOH:O	2.09	0.53
1:C:179:TYR:OH	1:C:455:ALA:HB2	2.09	0.53
1:A:221:LEU:HD21	1:A:240:VAL:HG11	1.90	0.53
1:A:371:MET:HE1	1:A:481:GLY:CA	2.38	0.53
1:C:161:ARG:HG3	1:C:463:PHE:HZ	1.73	0.53
1:A:191:VAL:HG12	1:A:192:ASN:N	2.24	0.53
1:C:172:LEU:HD23	1:C:176:PHE:CE2	2.44	0.53
1:A:243:ARG:O	1:A:247:ASN:CG	2.51	0.53
1:A:466:LYS:NZ	1:A:494:GLU:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HG21	1:B:456:LEU:HD11	1.91	0.53
1:A:189:PHE:HE2	1:A:303:ILE:HD11	1.74	0.52
1:B:443:ILE:HG22	2:B:601:HEM:HMD2	1.92	0.52
1:B:478:SER:HG	1:B:484:GLN:HB3	1.73	0.52
1:C:324:HIS:O	1:C:327:VAL:HG22	2.10	0.52
1:C:111:VAL:HG21	1:C:215:PHE:HZ	1.74	0.52
1:C:365:ARG:HA	1:C:402:HIS:ND1	2.25	0.52
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.40	0.52
1:B:132:LEU:HD21	1:B:288:LYS:HA	1.92	0.52
1:B:386:MET:HA	4:B:732:HOH:O	2.09	0.52
1:A:369:ILE:HA	1:A:483:LEU:HB3	1.92	0.52
1:A:261:LEU:HD12	1:A:264:THR:OG1	2.10	0.52
1:C:101:VAL:HG11	1:C:381:VAL:HG21	1.92	0.52
1:A:335:ILE:HA	1:A:353:MET:HE2	1.91	0.51
1:A:428:ASP:HB3	1:A:431:ILE:HG12	1.92	0.51
1:B:316:PHE:HE1	1:B:475:LEU:HD21	1.75	0.51
1:C:275:MET:HE1	1:C:298:GLN:HB2	1.91	0.51
1:B:179:TYR:CZ	1:B:455:ALA:HB2	2.45	0.51
1:C:183:VAL:HG11	1:C:451:ASN:ND2	2.25	0.51
1:A:261:LEU:CD1	1:A:264:THR:OG1	2.58	0.51
1:B:287:HIS:CD2	1:B:288:LYS:HB2	2.45	0.51
1:C:364:LEU:HD22	1:C:434:PRO:HB2	1.93	0.51
1:A:362:GLU:OE2	1:A:362:GLU:HA	2.11	0.51
1:B:342:LYS:O	1:B:458:ARG:NH1	2.44	0.51
1:C:221:LEU:HD21	1:C:240:VAL:CG1	2.41	0.51
1:B:423:ASN:HB3	1:B:426:ASN:HD21	1.76	0.51
1:A:371:MET:HE1	1:A:481:GLY:HA2	1.93	0.51
1:C:321:LEU:HB3	1:C:328:GLN:HE21	1.75	0.51
1:A:109:GLY:O	1:A:111:VAL:HG23	2.11	0.50
1:B:269:VAL:HG13	1:B:269:VAL:O	2.10	0.50
1:C:160:LEU:HD13	1:C:175:VAL:HG21	1.92	0.50
1:B:151:GLN:O	1:B:155:VAL:HG23	2.11	0.50
1:B:110:PRO:HG3	1:B:234:GLU:HG3	1.92	0.49
1:B:318:MET:HA	1:B:318:MET:HE2	1.94	0.49
1:A:156:LEU:HD13	1:A:179:TYR:HB2	1.94	0.49
1:C:84:ILE:HD12	1:C:89:MET:HB3	1.95	0.49
1:B:179:TYR:CE2	1:B:455:ALA:HB2	2.46	0.49
1:C:111:VAL:HG21	1:C:215:PHE:CE2	2.46	0.49
1:C:251:LYS:HG3	1:C:254:LYS:HD3	1.94	0.49
1:C:333:GLU:HA	1:C:335:ILE:HG22	1.94	0.49
1:C:413:LYS:CE	1:C:418:ARG:HD3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:PHE:CE1	1:C:394:VAL:HG21	2.48	0.49
1:B:287:HIS:CA	1:B:288:LYS:HB2	2.43	0.49
1:C:362:GLU:HG3	1:C:418:ARG:CZ	2.41	0.49
1:C:313:VAL:HB	1:C:452:MET:SD	2.53	0.49
1:A:184[A]:ILE:O	1:A:188:SER:HB2	2.12	0.48
1:A:184[A]:ILE:HG21	1:A:303:ILE:HA	1.95	0.48
1:A:477:LEU:HD13	1:A:483:LEU:HD11	1.95	0.48
1:B:89:MET:HE2	1:B:384:ASN:HB2	1.95	0.48
1:C:210:LEU:HD11	1:C:241:PHE:HZ	1.77	0.48
1:C:365:ARG:NH1	1:C:402:HIS:O	2.46	0.48
1:C:413:LYS:NZ	1:C:418:ARG:HD3	2.29	0.48
1:A:231:PRO:O	1:A:235:VAL:HG23	2.14	0.48
1:A:105:ARG:NH1	3:A:602:08J:H7	2.28	0.48
1:A:151:GLN:O	1:A:155:VAL:HG23	2.13	0.48
1:C:201:ASP:HB3	1:C:204:VAL:HG23	1.96	0.48
1:C:210:LEU:CD1	1:C:241:PHE:HZ	2.26	0.48
1:C:210:LEU:HD21	1:C:300:ILE:HG23	1.96	0.48
1:C:428:ASP:C	1:C:430:TYR:H	2.21	0.48
1:C:366:LEU:O	1:C:403:ARG:NH2	2.29	0.48
1:C:260:ARG:HG2	1:C:261:LEU:N	2.28	0.48
1:A:76:ASP:OD2	1:A:106:ARG:NH2	2.46	0.47
1:C:92:THR:HA	1:C:96:LYS:HB2	1.95	0.47
1:A:93:VAL:HG21	1:A:394:VAL:HG11	1.97	0.47
1:A:256:MET:O	1:A:260:ARG:HG3	2.14	0.47
1:B:305:ALA:HB2	3:B:602:08J:CAA	2.44	0.47
1:B:396:ILE:HD12	1:B:396:ILE:N	2.29	0.47
1:B:193:ILE:HG22	1:B:194:ASP:N	2.29	0.47
1:C:117:ALA:HB1	1:C:301:ILE:CG1	2.44	0.47
1:C:413:LYS:CD	1:C:418:ARG:HH11	2.27	0.47
2:C:601:HEM:C4D	3:C:602:08J:H3	2.49	0.47
1:B:370:ALA:O	1:B:371:MET:HB3	2.14	0.47
1:B:153:GLY:O	1:B:458:ARG:HG2	2.14	0.47
1:B:173:LYS:HD3	1:B:488:PRO:HG3	1.96	0.47
1:A:118:ILE:HD12	1:A:133:LEU:HD12	1.96	0.47
1:C:358:MET:HG2	1:C:419:PHE:HB3	1.96	0.47
1:C:413:LYS:HE3	1:C:418:ARG:HD3	1.96	0.47
1:B:287:HIS:CB	1:B:288:LYS:HB2	2.45	0.47
1:C:24:LEU:O	1:C:27:THR:HB	2.15	0.47
1:C:342:LYS:HA	1:C:461:GLN:NE2	2.30	0.47
1:C:309:THR:HG22	1:C:369:ILE:HD13	1.97	0.47
1:B:403:ARG:HA	1:B:411:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:SER:OG	1:C:494:GLU:HB2	2.15	0.47
1:A:104:ASN:HB2	4:A:731:HOH:O	2.14	0.46
1:A:186:SER:HA	1:A:191:VAL:O	2.15	0.46
1:B:93:VAL:HG21	1:B:394:VAL:HG11	1.96	0.46
1:C:128:ARG:NH1	1:C:289:ALA:O	2.47	0.46
1:C:369:ILE:CG1	3:C:602:08J:CLAC	2.93	0.46
1:B:145:MET:HE1	1:B:271:PHE:CD1	2.50	0.46
1:B:457:ILE:O	1:B:461:GLN:HG3	2.15	0.46
1:C:223:ILE:HD12	1:C:230:ILE:CG1	2.45	0.46
1:C:260:ARG:HB3	1:C:262:GLU:HB2	1.98	0.46
1:C:320:GLU:O	1:C:324:HIS:HB2	2.16	0.46
1:A:79:GLN:NE2	1:A:393:VAL:HG23	2.31	0.46
1:B:128:ARG:HH12	1:B:294:GLU:CD	2.24	0.46
1:C:50:ILE:HA	1:C:53:TYR:HD2	1.80	0.46
1:B:91:LYS:HG3	1:B:430:TYR:CZ	2.51	0.46
1:C:260:ARG:NH2	1:C:276:ILE:HG23	2.31	0.46
2:B:601:HEM:HHC	2:B:601:HEM:HBB2	1.98	0.46
1:C:58:CYS:SG	1:C:371:MET:HE2	2.56	0.46
1:C:257:LYS:HG3	1:C:276:ILE:HG12	1.97	0.46
1:C:93:VAL:HA	1:C:102:PHE:CD2	2.51	0.45
1:C:166:THR:HG22	1:C:166:THR:O	2.15	0.45
1:A:221:LEU:HD12	1:A:223:ILE:HD11	1.98	0.45
1:A:309:THR:CG2	3:A:602:08J:CLAC	3.02	0.45
1:A:403:ARG:NH1	1:A:412:GLU:OE1	2.48	0.45
1:C:117:ALA:HB1	1:C:301:ILE:HG13	1.98	0.45
1:C:346:THR:O	1:C:347:TYR:C	2.59	0.45
1:A:111:VAL:HG12	1:A:111:VAL:O	2.15	0.45
1:B:130:ARG:NH1	2:B:601:HEM:O1D	2.50	0.45
1:B:134:SER:HB3	1:B:135:PRO:HD3	1.97	0.45
1:B:157:VAL:HG23	1:B:463:PHE:CZ	2.51	0.45
1:C:119:SER:OG	3:C:602:08J:NAN	2.44	0.45
1:C:468:CYS:SG	1:C:469:LYS:N	2.89	0.45
1:A:144:GLU:O	1:A:269:VAL:HG11	2.15	0.45
1:B:288:LYS:HG2	1:B:289:ALA:N	2.32	0.45
1:B:426:ASN:N	1:B:426:ASN:OD1	2.50	0.45
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.97	0.45
1:A:263:ASP:HB2	1:C:158:ARG:NH1	2.32	0.45
1:C:316:PHE:HB3	1:C:363:THR:HG23	1.98	0.45
1:A:350:VAL:HG21	1:A:454:LEU:HD23	1.98	0.45
1:C:209:LYS:HG3	1:C:212:ARG:NH2	2.32	0.45
1:C:256:MET:C	1:C:260:ARG:HA	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:HE1	1:A:480:GLY:O	2.17	0.45
1:B:318:MET:HE1	1:B:321:LEU:HD12	1.99	0.44
1:C:39:PRO:HG2	1:C:68:TYR:HB3	1.99	0.44
1:A:120:ILE:HD11	1:A:215:PHE:HE2	1.83	0.44
1:A:256:MET:N	4:A:701:HOH:O	2.50	0.44
1:A:120:ILE:HD11	1:A:215:PHE:CE2	2.52	0.44
1:A:211:LEU:HD21	1:A:303:ILE:HG22	1.99	0.44
1:B:301:ILE:HD12	1:B:301:ILE:HA	1.86	0.44
1:B:386:MET:HE3	1:B:388:ILE:HD11	2.00	0.44
1:A:148:ILE:HD12	1:A:148:ILE:H	1.83	0.44
1:A:193:ILE:HG22	1:A:194:ASP:H	1.81	0.44
1:C:161:ARG:CG	1:C:463:PHE:HZ	2.30	0.44
1:C:344:PRO:HA	1:C:345:PRO:HD3	1.84	0.44
1:C:71:VAL:HG21	1:C:386:MET:SD	2.58	0.44
1:A:193:ILE:HG22	1:A:194:ASP:N	2.32	0.44
1:A:40:GLY:HA3	1:A:73:GLY:O	2.18	0.44
1:A:254:LYS:C	4:A:701:HOH:O	2.61	0.43
1:A:305:ALA:HB2	3:A:602:08J:H5	2.00	0.43
1:C:62:MET:HE1	1:C:403:ARG:HB2	2.01	0.43
1:A:259:SER:O	1:A:263:ASP:HB3	2.17	0.43
1:B:138:THR:OG1	1:B:141:LYS:HG2	2.18	0.43
1:C:145:MET:HE1	1:C:271:PHE:CD1	2.54	0.43
1:C:370:ALA:C	1:C:372:ARG:H	2.25	0.43
1:B:159:ASN:HA	1:B:162:ARG:HD2	2.00	0.43
1:B:243:ARG:HG2	1:B:247:ASN:HD21	1.84	0.43
1:B:83:ALA:HA	1:B:395:MET:O	2.19	0.43
1:C:456:LEU:O	1:C:459:VAL:HG22	2.18	0.43
1:C:468:CYS:C	1:C:470:GLU:H	2.26	0.43
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.46	0.43
1:A:91:LYS:NZ	4:A:707:HOH:O	2.51	0.43
1:B:257:LYS:HG2	1:B:276:ILE:HD11	1.99	0.43
1:A:252:SER:O	1:A:255:ARG:HG2	2.19	0.43
1:A:330:LYS:HD3	1:A:355:TYR:CZ	2.54	0.43
1:B:383:ILE:O	1:B:383:ILE:HG13	2.19	0.43
1:C:152:TYR:OH	1:C:186:SER:HB3	2.18	0.43
1:C:331:LEU:HD12	1:C:355:TYR:HB3	2.01	0.43
1:A:27:THR:CG2	1:A:28:HIS:N	2.81	0.43
1:A:186:SER:O	1:A:190:GLY:HA2	2.19	0.43
1:A:252:SER:O	1:A:256:MET:HG3	2.19	0.42
1:B:194:ASP:OD2	1:B:197:ASN:HB2	2.18	0.42
1:C:294:GLU:O	1:C:298:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ALA:HA	1:C:344:PRO:HD3	1.94	0.42
1:A:111:VAL:HG11	1:A:215:PHE:HZ	1.84	0.42
1:A:275:MET:HB3	1:A:295:LEU:CD1	2.49	0.42
1:C:223:ILE:HD13	1:C:229:LEU:HD23	2.01	0.42
1:C:419:PHE:CA	1:C:424:LYS:HG3	2.49	0.42
1:A:133:LEU:HD11	1:A:298:GLN:HE21	1.85	0.42
1:A:309:THR:HG22	3:A:602:08J:CLAC	2.56	0.42
1:C:172:LEU:HD23	1:C:176:PHE:HE2	1.84	0.42
1:C:189:PHE:CZ	1:C:249:LEU:HD23	2.54	0.42
1:C:257:LYS:O	1:C:257:LYS:HG2	2.18	0.42
1:C:331:LEU:HD12	1:C:355:TYR:HD2	1.82	0.42
1:B:287:HIS:HA	1:B:288:LYS:HB2	2.01	0.42
1:A:298:GLN:O	1:A:301:ILE:HG22	2.19	0.42
1:C:413:LYS:HE3	1:C:418:ARG:CD	2.49	0.42
1:C:111:VAL:HG23	1:C:241:PHE:HB3	2.02	0.42
1:C:111:VAL:HG23	1:C:241:PHE:CB	2.50	0.42
1:C:130:ARG:HD2	1:C:443:ILE:HD12	2.02	0.42
1:B:318:MET:HE3	1:B:456:LEU:HD22	2.02	0.42
1:C:265:GLN:HE21	1:C:267:HIS:HB2	1.85	0.42
1:A:410:GLU:OE2	1:A:413:LYS:HE3	2.20	0.42
1:B:50:ILE:O	1:B:53:TYR:HB2	2.20	0.42
1:B:318:MET:CE	1:B:321:LEU:HD12	2.50	0.42
1:A:344:PRO:HA	1:A:345:PRO:HD3	1.92	0.42
1:B:221:LEU:HD11	1:B:240:VAL:HG21	2.02	0.42
1:C:362:GLU:HG3	4:C:701:HOH:O	2.19	0.42
1:C:420:SER:O	1:C:424:LYS:HE2	2.20	0.42
1:C:405:PRO:HA	1:C:411:PRO:HG3	2.02	0.41
1:B:338:VAL:CG1	1:B:353:MET:HE2	2.50	0.41
1:C:161:ARG:HG3	1:C:463:PHE:CZ	2.54	0.41
1:A:356:LEU:HD21	1:A:453:LYS:HB3	2.02	0.41
1:B:187:THR:O	1:B:271:PHE:N	2.36	0.41
1:A:260:ARG:HD3	1:A:273:GLN:OE1	2.20	0.41
1:B:106:ARG:HH11	1:B:374:GLU:CD	2.28	0.41
1:C:131:SER:C	1:C:133:LEU:H	2.28	0.41
1:A:184[A]:ILE:HD11	1:A:307:TYR:HA	2.02	0.41
1:A:492:LYS:NZ	4:A:711:HOH:O	2.54	0.41
1:A:496:ARG:O	1:A:497:ASP:CB	2.69	0.41
1:C:52:SER:HB3	1:C:60:PHE:CD1	2.55	0.41
1:A:133:LEU:HD11	1:A:298:GLN:NE2	2.35	0.41
1:A:365:ARG:O	1:A:402:HIS:HB3	2.21	0.41
1:B:372:ARG:HG2	1:B:395:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LYS:HA	1:B:413:LYS:HD2	1.97	0.41
1:C:300:ILE:HA	1:C:303:ILE:HD12	2.03	0.41
1:B:264:THR:O	1:B:266:LYS:HG3	2.21	0.41
1:B:421:LYS:C	1:B:423:ASN:H	2.29	0.41
1:C:58:CYS:SG	1:C:371:MET:HG2	2.61	0.41
1:C:324:HIS:CE1	1:C:414:PHE:HB3	2.56	0.41
1:C:118:ILE:HD12	1:C:133:LEU:HD12	2.03	0.41
1:B:89:MET:HE3	1:B:89:MET:HB2	1.95	0.40
1:B:254:LYS:HB2	1:B:254:LYS:HE3	1.89	0.40
1:C:230:ILE:HB	1:C:231:PRO:CD	2.51	0.40
1:A:57:PHE:N	1:A:57:PHE:CD1	2.89	0.40
1:A:184[B]:ILE:CG2	1:A:303:ILE:HG12	2.51	0.40
1:A:241:PHE:HA	1:A:242:PRO:HD3	1.85	0.40
1:B:255:ARG:O	1:B:259:SER:OG	2.22	0.40
1:B:421:LYS:C	1:B:423:ASN:N	2.77	0.40
1:C:102:PHE:HE1	1:C:394:VAL:HG21	1.84	0.40
1:C:415:LEU:H	1:C:418:ARG:NH1	2.15	0.40
1:A:191:VAL:CG1	1:A:192:ASN:N	2.83	0.40
1:A:216:LEU:HD13	3:A:602:08J:CAR	2.52	0.40
1:C:111:VAL:HG22	1:C:111:VAL:O	2.22	0.40
1:C:159:ASN:O	1:C:162:ARG:CB	2.70	0.40
1:C:253:VAL:O	1:C:257:LYS:N	2.55	0.40
1:C:413:LYS:HZ1	1:C:418:ARG:HD3	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLU:OE2	1:C:466:LYS:CE[4_545]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/487 (96%)	435 (94%)	29 (6%)	1 (0%)	43	68
1	B	467/487 (96%)	424 (91%)	43 (9%)	0	100	100
1	C	465/487 (96%)	402 (86%)	62 (13%)	1 (0%)	43	68
All	All	1397/1461 (96%)	1261 (90%)	134 (10%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ARG
1	C	347	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/443 (97%)	415 (96%)	15 (4%)	32	61
1	B	430/443 (97%)	415 (96%)	15 (4%)	32	61
1	C	428/443 (97%)	404 (94%)	24 (6%)	19	44
All	All	1288/1329 (97%)	1234 (96%)	54 (4%)	26	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	42	THR
1	A	175	VAL
1	A	188	SER
1	A	193	ILE
1	A	210	LEU
1	A	222	SER
1	A	225	VAL
1	A	275	MET
1	A	288	LYS
1	A	291	SER

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Mol	Chain	Res	Type
1	A	372	ARG
1	A	425	ASP
1	A	466	LYS
1	A	469	LYS
1	B	27	THR
1	B	34	LYS
1	B	51	LEU
1	B	101	VAL
1	B	141	LYS
1	B	188	SER
1	B	225	VAL
1	B	269	VAL
1	B	274	LEU
1	B	301	ILE
1	B	371	MET
1	B	421	LYS
1	B	458	ARG
1	B	475	LEU
1	B	494	GLU
1	C	27	THR
1	C	63	GLU
1	C	104	ASN
1	C	143	LYS
1	C	149	ILE
1	C	191	VAL
1	C	203	PHE
1	C	225	VAL
1	C	258	GLU
1	C	261	LEU
1	C	264	THR
1	C	294	GLU
1	C	301	ILE
1	C	315	SER
1	C	331	LEU
1	C	351	LEU
1	C	362	GLU
1	C	380	ASP
1	C	422	LYS
1	C	427	ILE
1	C	454	LEU
1	C	460	LEU
1	C	477	LEU

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Mol	Chain	Res	Type
1	C	492	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	65	HIS
1	A	287	HIS
1	A	298	GLN
1	A	332	GLN
1	A	423	ASN
1	A	461	GLN
1	B	198	ASN
1	B	287	HIS
1	B	341	ASN
1	C	151	GLN
1	C	265	GLN
1	C	273	GLN
1	C	279	GLN
1	C	324	HIS
1	C	328	GLN
1	C	461	GLN
1	C	472	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	B	601	1	50,50,50	1.64	9 (18%)	67,82,82	1.59	15 (22%)
3	08J	C	602	-	26,26,26	1.76	5 (19%)	33,38,38	7.81	17 (51%)
3	08J	B	602	-	26,26,26	1.60	5 (19%)	33,38,38	2.78	13 (39%)
3	08J	A	602	-	26,26,26	1.65	5 (19%)	33,38,38	4.62	14 (42%)
2	HEM	C	601	1	50,50,50	1.59	8 (16%)	67,82,82	1.56	11 (16%)
2	HEM	A	601	1	50,50,50	1.62	9 (18%)	67,82,82	1.58	14 (20%)

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	1	-	4/14/54/54	-
3	08J	C	602	-	-	0/2/17/17	1/4/4/4
3	08J	B	602	-	-	0/2/17/17	0/4/4/4
3	08J	A	602	-	-	0/2/17/17	0/4/4/4
2	HEM	C	601	1	-	3/14/54/54	-
2	HEM	A	601	1	-	2/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	FE-NB	5.73	2.12	1.94
2	A	601	HEM	FE-NC	5.07	2.11	1.95
3	C	602	08J	CAO-NAM	-4.97	1.22	1.28
2	A	601	HEM	FE-NB	4.92	2.10	1.94
2	C	601	HEM	FE-NB	4.76	2.09	1.94
3	A	602	08J	CAV-NAW	-4.46	1.36	1.44
3	B	602	08J	CAV-NAW	-4.31	1.36	1.44
2	C	601	HEM	FE-NC	4.22	2.09	1.95
3	C	602	08J	CAL-NAM	-4.17	1.40	1.47
2	B	601	HEM	FE-NC	4.15	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	08J	CAS-NAW	-3.84	1.34	1.40
3	A	602	08J	CAL-NAM	3.63	1.53	1.47
2	C	601	HEM	C1B-NB	-3.13	1.34	1.40
2	A	601	HEM	C1B-NB	-3.13	1.34	1.40
2	B	601	HEM	C1B-NB	-3.10	1.34	1.40
2	C	601	HEM	C4B-NB	-2.93	1.33	1.38
2	C	601	HEM	C4D-ND	-2.85	1.35	1.40
2	C	601	HEM	C1D-ND	-2.84	1.33	1.38
2	B	601	HEM	C4D-ND	-2.81	1.35	1.40
3	C	602	08J	CAV-NAW	-2.80	1.39	1.44
2	A	601	HEM	C4B-NB	-2.75	1.33	1.38
2	A	601	HEM	C4D-ND	-2.70	1.35	1.40
3	A	602	08J	CAS-NAW	-2.66	1.36	1.40
2	B	601	HEM	C3C-C4C	-2.62	1.41	1.46
3	C	602	08J	CAL-CAS	2.60	1.53	1.48
2	B	601	HEM	C1D-ND	-2.58	1.33	1.38
3	B	602	08J	CAR-NAW	-2.57	1.34	1.38
3	A	602	08J	CAR-NAW	-2.57	1.34	1.38
2	A	601	HEM	C1D-ND	-2.53	1.33	1.38
2	C	601	HEM	C3C-C4C	-2.29	1.42	1.46
2	B	601	HEM	C1C-C2C	-2.23	1.40	1.45
2	B	601	HEM	C4B-NB	-2.18	1.34	1.38
2	B	601	HEM	C4A-NA	-2.13	1.35	1.39
2	A	601	HEM	C1C-C2C	-2.11	1.41	1.45
3	B	602	08J	CAP-CLAC	2.07	1.79	1.74
3	B	602	08J	CAO-NAM	-2.06	1.26	1.28
2	A	601	HEM	C4A-NA	-2.06	1.35	1.39
2	A	601	HEM	C3C-C4C	-2.04	1.42	1.46
2	C	601	HEM	FE-ND	-2.02	1.88	1.94
3	C	602	08J	CAR-NAW	-2.00	1.35	1.38
3	A	602	08J	CAO-NAM	-2.00	1.26	1.28

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	08J	CAL-NAM-CAO	32.12	153.83	117.46
3	A	602	08J	CAL-NAM-CAO	19.78	139.87	117.46
3	C	602	08J	CAU-CAO-NAM	-17.31	96.73	125.06
3	C	602	08J	CAV-NAW-CAR	-13.91	120.15	130.92
3	C	602	08J	CAT-CAO-NAM	12.89	134.26	116.84
3	A	602	08J	CAV-NAW-CAR	-9.96	123.21	130.92
3	B	602	08J	CAL-NAM-CAO	9.30	127.99	117.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	08J	CAT-CAO-CAU	8.04	128.89	117.62
3	C	602	08J	CAV-CAU-CAO	-7.96	111.83	122.72
3	C	602	08J	CAK-CAU-CAV	6.12	125.97	118.76
3	A	602	08J	CAU-CAO-NAM	-5.93	115.36	125.06
3	A	602	08J	NAW-CAR-NAN	-5.88	104.91	111.87
3	B	602	08J	CAV-NAW-CAR	-5.81	126.42	130.92
3	B	602	08J	NAW-CAR-NAN	-5.17	105.75	111.87
2	A	601	HEM	CHC-C4B-NB	5.15	129.97	124.42
3	C	602	08J	CAU-CAV-NAW	5.07	128.57	120.31
3	C	602	08J	NAW-CAR-NAN	-4.96	106.00	111.87
3	A	602	08J	CAK-CAU-CAV	4.89	124.52	118.76
3	A	602	08J	CAJ-NAN-CAR	4.81	110.53	106.03
3	C	602	08J	CAI-CAV-CAU	-4.38	112.43	119.16
2	C	601	HEM	CHC-C4B-NB	4.38	129.14	124.42
2	C	601	HEM	CHB-C1B-NB	4.32	129.71	124.37
3	C	602	08J	CAV-NAW-CAS	4.21	128.34	121.32
3	C	602	08J	CAJ-NAN-CAR	4.20	109.96	106.03
2	C	601	HEM	C1B-NB-C4B	4.06	110.01	105.21
2	B	601	HEM	CHD-C4C-NC	4.01	128.82	124.45
3	A	602	08J	CAA-CAR-NAW	3.98	130.62	123.97
3	B	602	08J	CAA-CAR-NAW	3.91	130.51	123.97
3	B	602	08J	CAJ-NAN-CAR	3.87	109.65	106.03
2	B	601	HEM	CHB-C1B-NB	3.85	129.13	124.37
2	C	601	HEM	CHA-C4D-ND	3.84	129.12	124.37
2	B	601	HEM	C1B-NB-C4B	3.79	109.69	105.21
2	A	601	HEM	C1B-NB-C4B	3.70	109.59	105.21
2	A	601	HEM	CHB-C1B-NB	3.65	128.89	124.37
3	A	602	08J	CAT-CAO-NAM	3.53	121.61	116.84
3	C	602	08J	CAA-CAR-NAW	3.45	129.75	123.97
2	A	601	HEM	CHD-C1D-ND	3.39	128.07	124.42
2	B	601	HEM	CHC-C4B-NB	3.35	128.03	124.42
3	B	602	08J	CAI-CAV-CAU	-3.30	114.09	119.16
3	A	602	08J	CAI-CAV-CAU	-3.25	114.17	119.16
2	B	601	HEM	CHA-C4D-ND	3.22	128.35	124.37
2	A	601	HEM	CHA-C4D-ND	3.08	128.18	124.37
3	B	602	08J	CAK-CAU-CAO	-2.94	114.58	118.87
3	A	602	08J	CAG-CAT-CAQ	2.92	119.95	116.70
2	C	601	HEM	CHA-C4D-C3D	-2.85	119.96	125.23
2	B	601	HEM	CHD-C1D-ND	2.83	127.47	124.42
3	B	602	08J	CAH-CAI-CAV	2.83	124.78	119.10
3	B	602	08J	CAK-CAU-CAV	2.82	122.08	118.76
2	C	601	HEM	CHD-C4C-NC	2.81	127.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	08J	CAV-CAU-CAO	-2.80	118.89	122.72
3	C	602	08J	CAG-CAT-CAQ	2.80	119.81	116.70
2	B	601	HEM	C3B-C4B-NB	-2.79	107.46	109.47
2	C	601	HEM	CHD-C1D-ND	2.79	127.42	124.42
3	B	602	08J	CAU-CAV-NAW	2.77	124.83	120.31
2	A	601	HEM	CHD-C1D-C2D	-2.76	120.66	125.03
2	C	601	HEM	O2A-CGA-CBA	2.69	122.49	114.00
2	C	601	HEM	C3B-C4B-NB	-2.68	107.54	109.47
2	A	601	HEM	CHA-C4D-C3D	-2.52	120.57	125.23
3	C	602	08J	CAH-CAI-CAV	2.50	124.11	119.10
3	A	602	08J	CAT-CAO-CAU	2.47	121.09	117.62
2	A	601	HEM	O2A-CGA-CBA	2.47	121.81	114.00
2	B	601	HEM	O2D-CGD-CBD	2.46	121.77	114.00
2	C	601	HEM	O2D-CGD-CBD	2.42	121.65	114.00
2	A	601	HEM	CBA-CAA-C2A	-2.42	105.84	112.53
2	B	601	HEM	O2A-CGA-CBA	2.41	121.62	114.00
2	A	601	HEM	O2D-CGD-CBD	2.41	121.62	114.00
2	A	601	HEM	C3B-C4B-NB	-2.40	107.75	109.47
2	B	601	HEM	CHA-C4D-C3D	-2.37	120.85	125.23
3	B	602	08J	CAU-CAO-NAM	-2.37	121.18	125.06
2	B	601	HEM	C4C-NC-C1C	2.31	109.58	105.82
3	A	602	08J	CAU-CAV-NAW	2.30	124.06	120.31
2	C	601	HEM	CHB-C1B-C2B	-2.29	120.43	126.95
3	C	602	08J	CAK-CAU-CAO	2.27	122.18	118.87
3	C	602	08J	CAF-CAQ-CAT	-2.25	120.64	123.07
3	B	602	08J	CAG-CAT-CAQ	2.24	119.19	116.70
2	A	601	HEM	CHD-C4C-NC	2.24	126.89	124.45
2	B	601	HEM	CAD-C3D-C4D	2.12	128.39	124.70
2	A	601	HEM	CHA-C1A-NA	2.09	127.66	123.86
3	B	602	08J	CAT-CAO-CAU	2.09	120.55	117.62
2	A	601	HEM	CHB-C1B-C2B	-2.07	121.07	126.95
2	B	601	HEM	CHB-C1B-C2B	-2.07	121.07	126.95
3	A	602	08J	CAH-CAP-CLAC	2.07	122.41	119.36
2	B	601	HEM	C4C-CHD-C1D	-2.05	121.67	126.02
2	B	601	HEM	CHD-C1D-C2D	-2.05	121.80	125.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	C2D-C3D-CAD-CBD
2	C	601	HEM	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	B	601	HEM	C2C-C3C-CAC-CBC
2	B	601	HEM	C4C-C3C-CAC-CBC
2	B	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	C2B-C3B-CAB-CBB
2	A	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAA-CBA-CGA-O2A

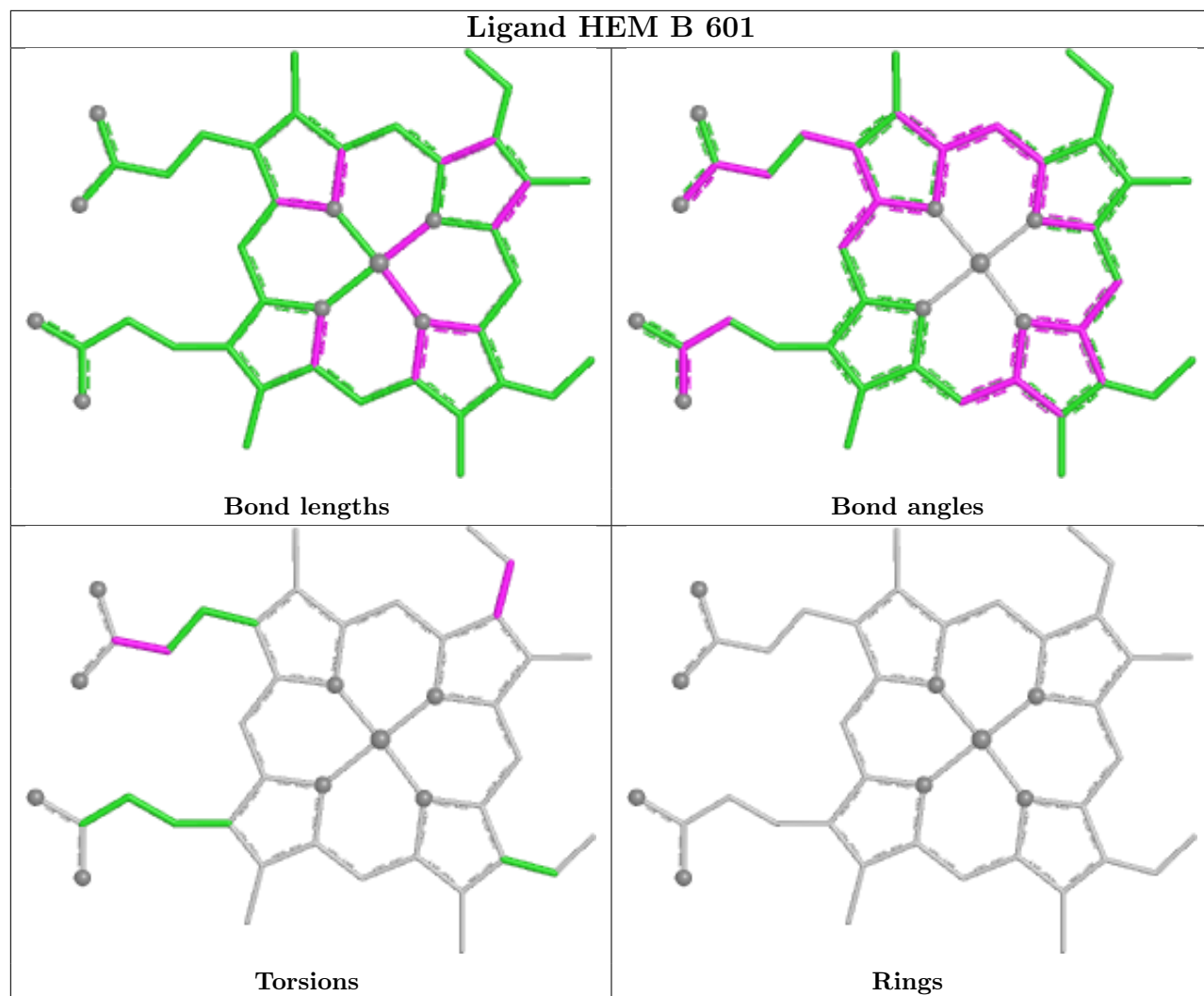
All (1) ring outliers are listed below:

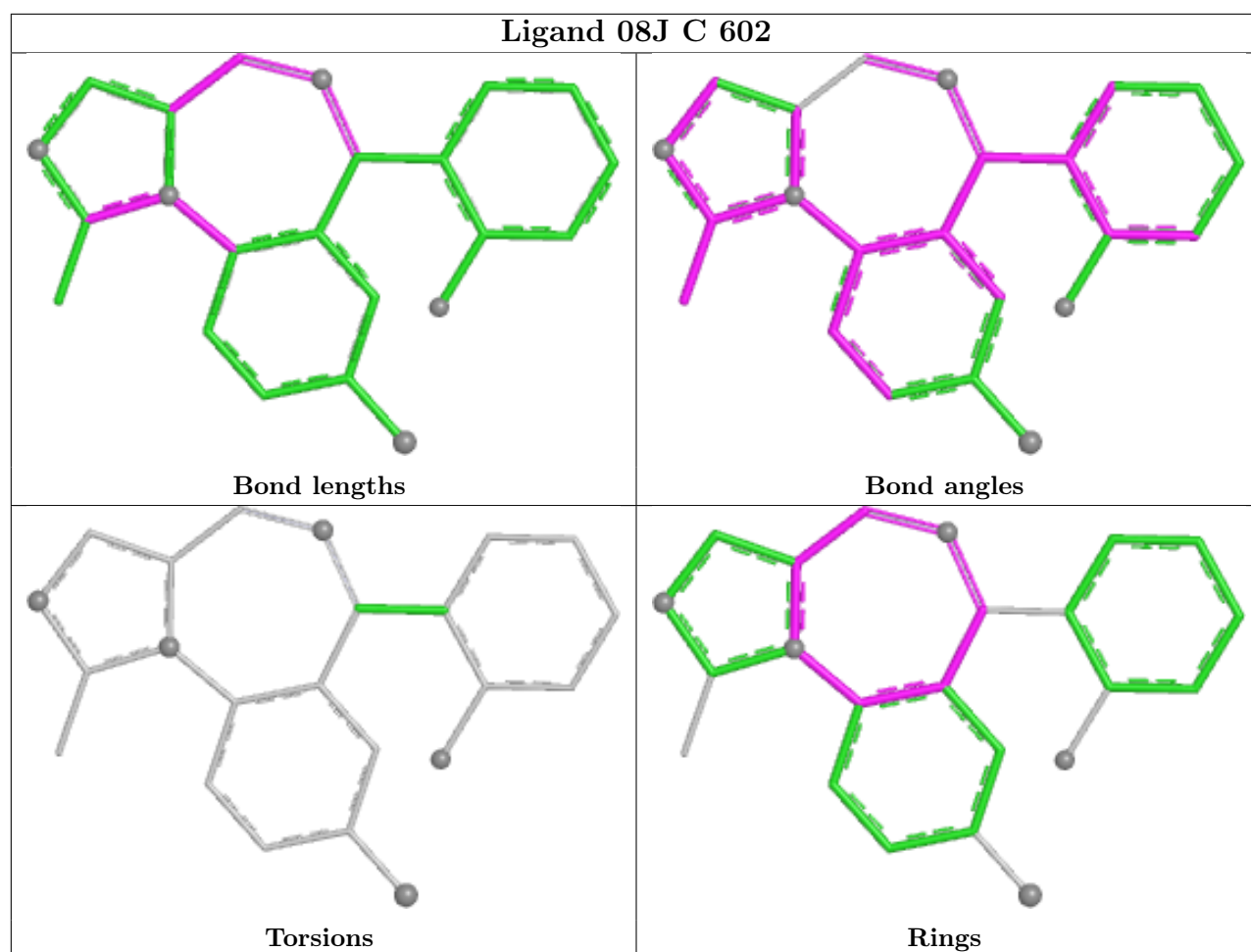
Mol	Chain	Res	Type	Atoms
3	C	602	08J	CAL-CAO-CAS-CAU-CAV-NAM-NAW

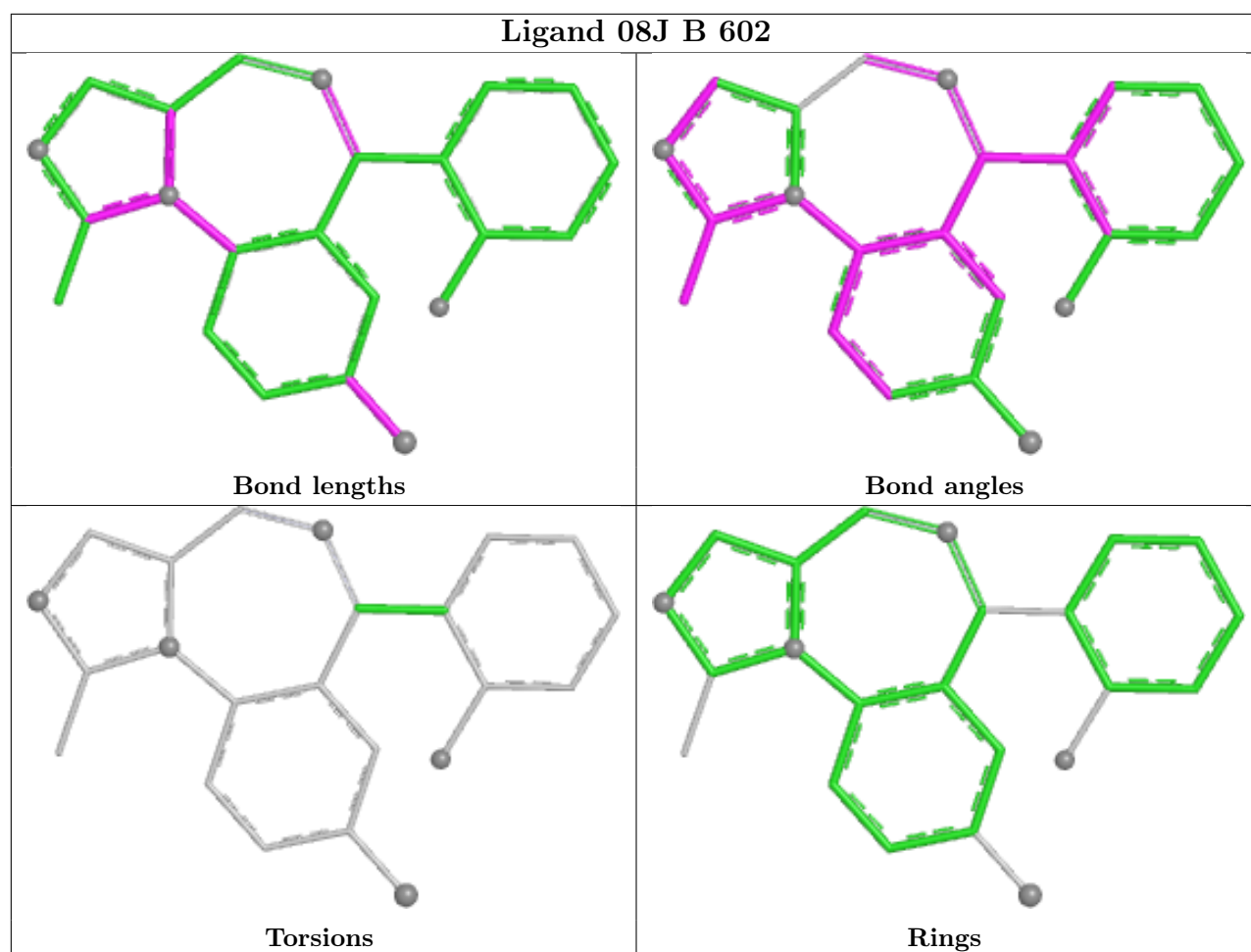
6 monomers are involved in 30 short contacts:

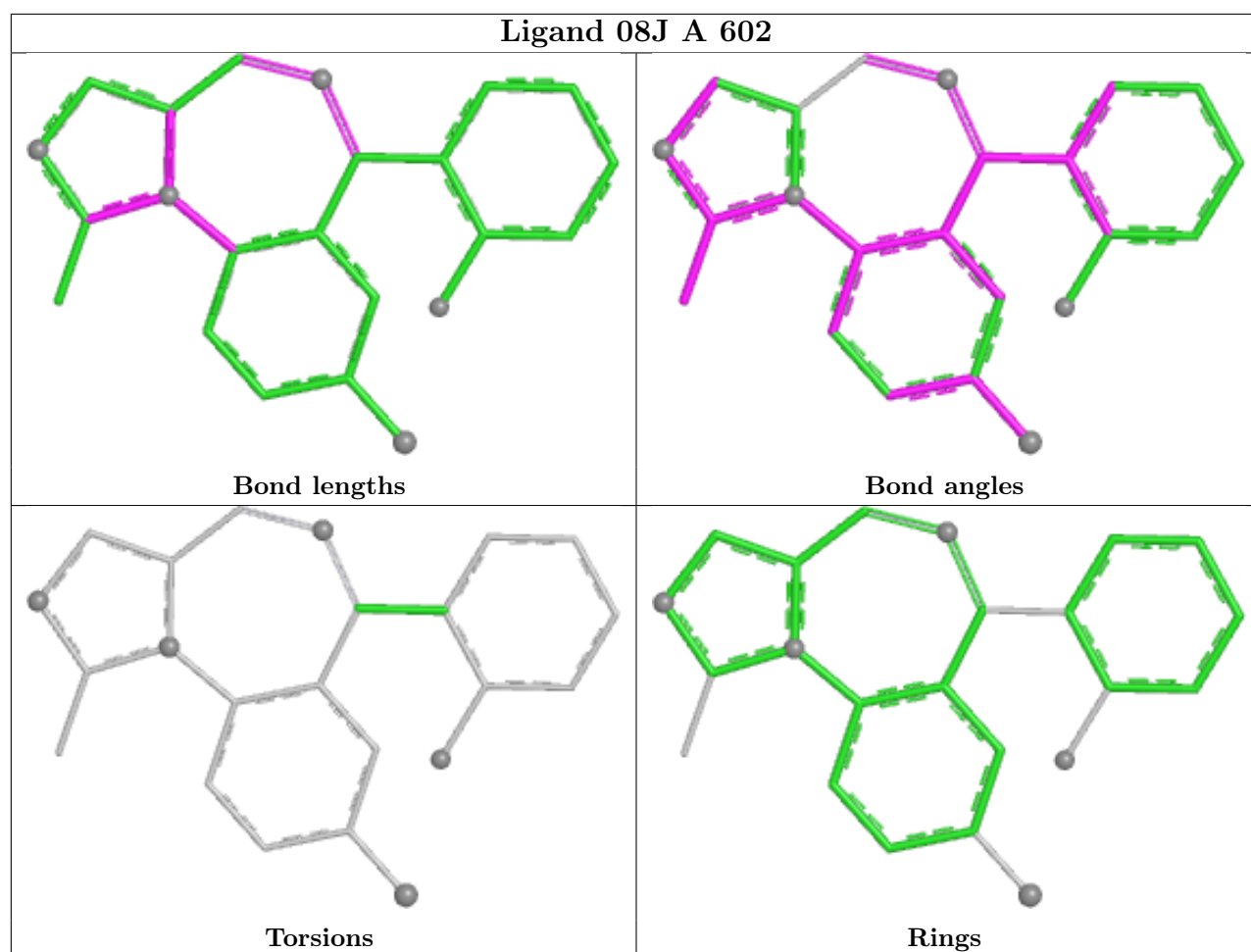
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	3	0
3	C	602	08J	12	0
3	B	602	08J	1	0
3	A	602	08J	7	0
2	C	601	HEM	6	0
2	A	601	HEM	3	0

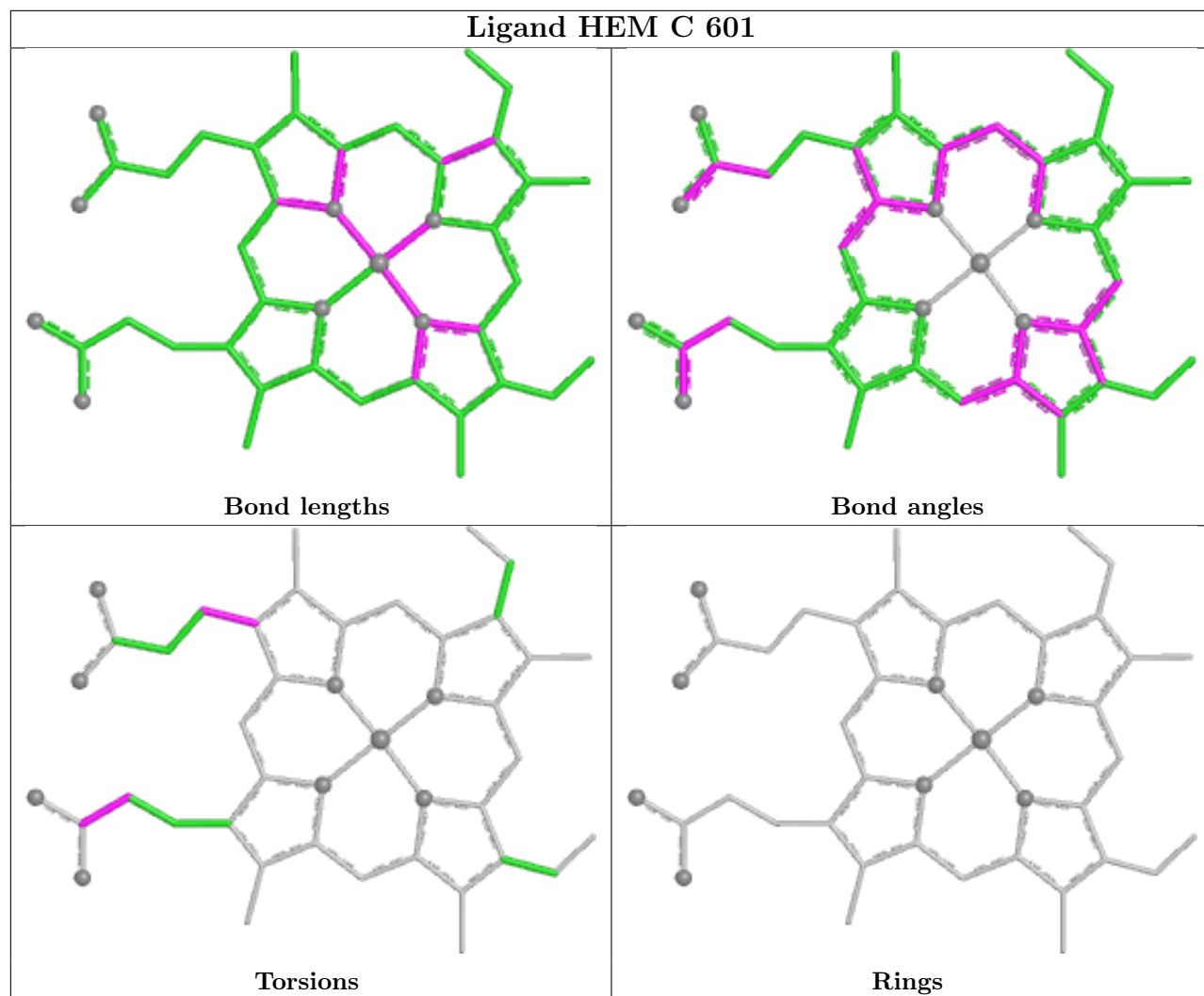
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

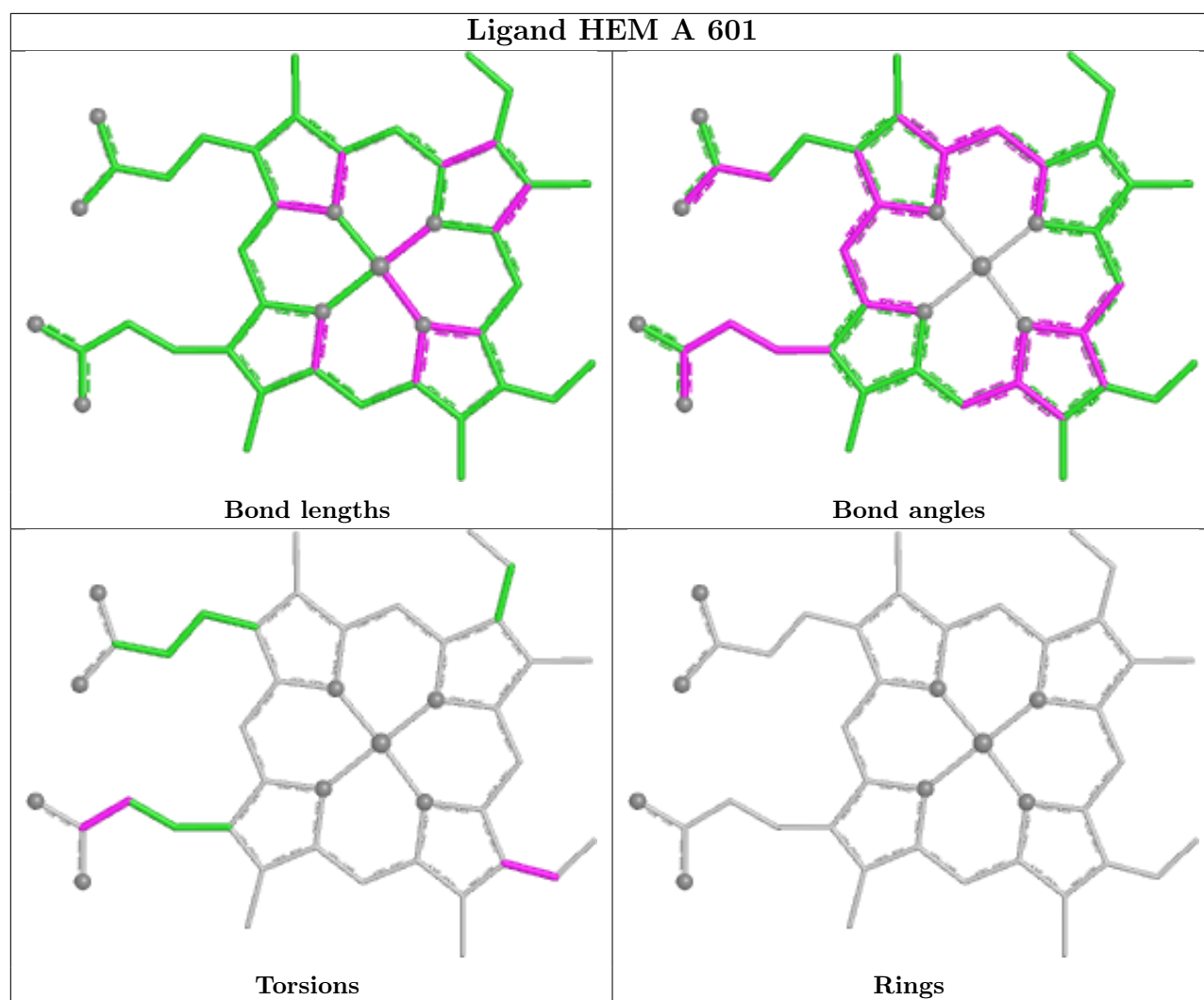












5.7 Other polymers [i](#)

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	470/487 (96%)	0.05	10 (2%) 63 61	25, 48, 90, 163	1 (0%)
1	B	471/487 (96%)	0.36	17 (3%) 46 42	25, 63, 121, 167	0
1	C	469/487 (96%)	0.91	49 (10%) 11 10	38, 96, 163, 186	0
All	All	1410/1461 (96%)	0.44	76 (5%) 31 27	25, 65, 145, 186	1 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	350	VAL	3.6
1	B	287	HIS	3.4
1	C	454	LEU	3.2
1	B	497	ASP	3.2
1	A	185	THR	3.0
1	C	162	ARG	3.0
1	A	281	SER	3.0
1	B	261	LEU	2.9
1	C	345	PRO	2.9
1	B	470	GLU	2.8
1	C	328	GLN	2.8
1	A	269	VAL	2.8
1	B	203	PHE	2.8
1	B	281	SER	2.8
1	C	288	LYS	2.8
1	C	290	LEU	2.8
1	C	323	THR	2.7
1	A	266	LYS	2.7
1	C	360	VAL	2.7
1	C	347	TYR	2.6
1	C	321	LEU	2.6
1	B	468	CYS	2.6
1	C	264	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	337	ALA	2.5
1	C	420	SER	2.5
1	B	255	ARG	2.5
1	B	240	VAL	2.5
1	B	264	THR	2.5
1	C	363	THR	2.5
1	A	184[A]	ILE	2.5
1	C	228	PHE	2.5
1	C	419	PHE	2.5
1	C	493	VAL	2.4
1	C	189	PHE	2.4
1	C	322	ALA	2.4
1	C	263	ASP	2.4
1	C	469	LYS	2.4
1	A	193	ILE	2.3
1	C	408	TRP	2.3
1	B	108	PHE	2.3
1	C	167	GLY	2.3
1	C	132	LEU	2.3
1	C	319	TYR	2.3
1	C	465	PHE	2.3
1	C	289	ALA	2.2
1	B	244	GLU	2.2
1	C	99	TYR	2.2
1	C	385	GLY	2.2
1	B	160	LEU	2.2
1	C	351	LEU	2.2
1	C	346	THR	2.2
1	C	475	LEU	2.2
1	C	316	PHE	2.2
1	C	379	LYS	2.2
1	A	261	LEU	2.2
1	C	335	ILE	2.2
1	A	258	GLU	2.1
1	C	268	ARG	2.1
1	C	173	LYS	2.1
1	C	415	LEU	2.1
1	C	456	LEU	2.1
1	C	348	ASP	2.1
1	B	2	ALA	2.1
1	B	266	LYS	2.1
1	C	249	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	268	ARG	2.1
1	C	416	PRO	2.1
1	B	249	LEU	2.1
1	A	264	THR	2.1
1	A	267	HIS	2.1
1	C	193	ILE	2.1
1	C	161	ARG	2.0
1	C	333	GLU	2.0
1	C	196	LEU	2.0
1	C	490	VAL	2.0
1	C	355	TYR	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](#)

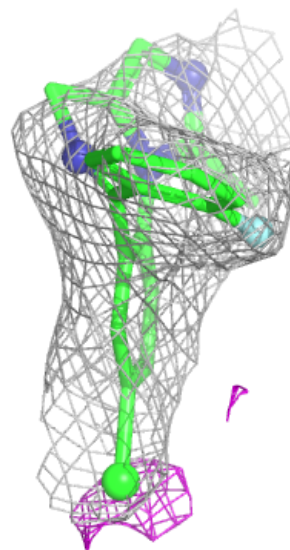
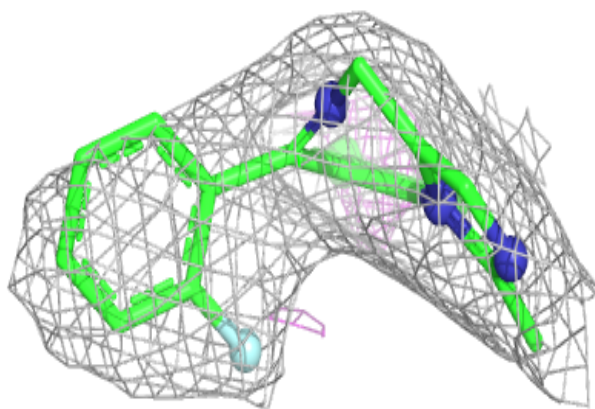
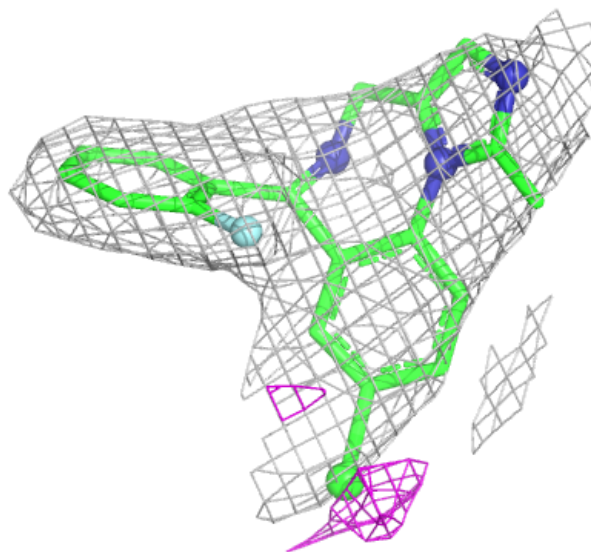
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	08J	C	602	23/23	0.85	0.14	73,87,95,115	0
3	08J	A	602	23/23	0.93	0.09	32,34,37,37	0
3	08J	B	602	23/23	0.95	0.07	39,40,42,44	0
2	HEM	C	601	43/43	0.95	0.11	58,62,67,70	0
2	HEM	B	601	43/43	0.97	0.07	29,37,41,45	0
2	HEM	A	601	43/43	0.98	0.06	22,25,30,31	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.

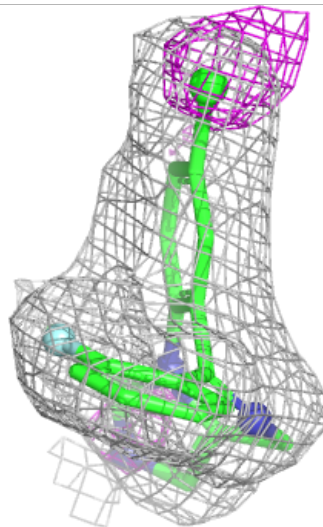
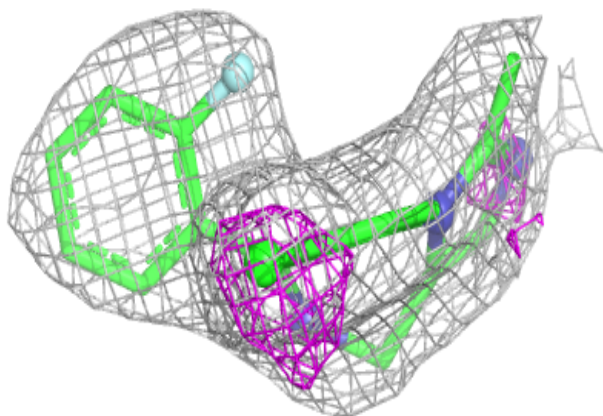
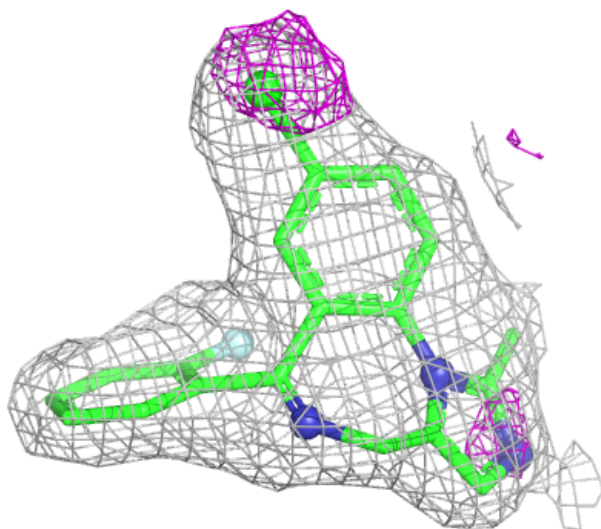
Electron density around 08J C 602:

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



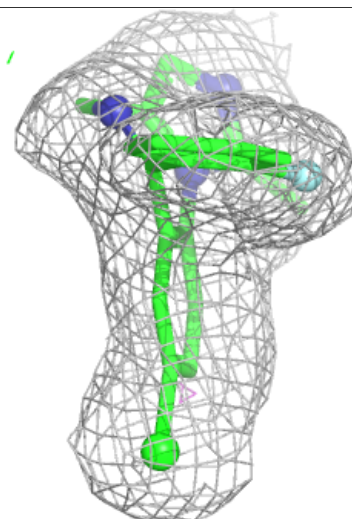
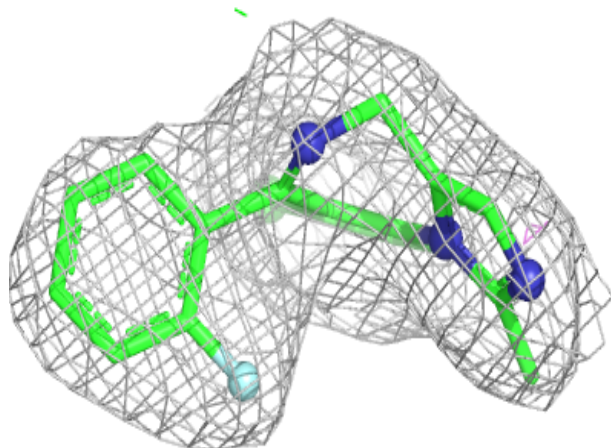
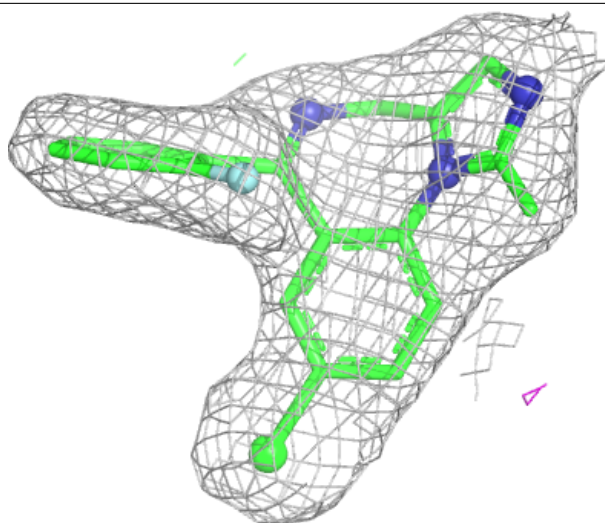
Electron density around 08J A 602:

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



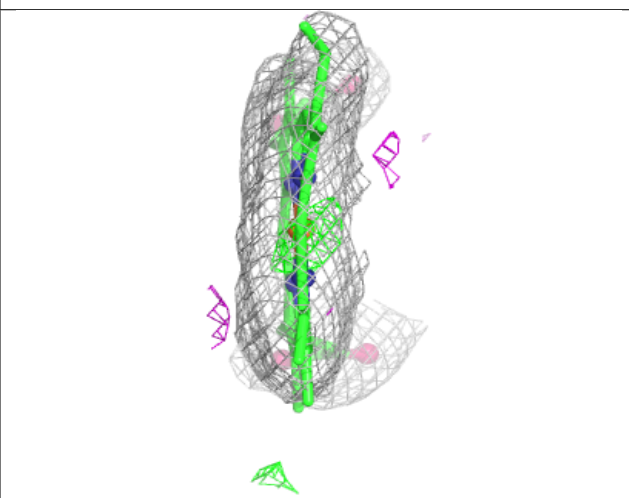
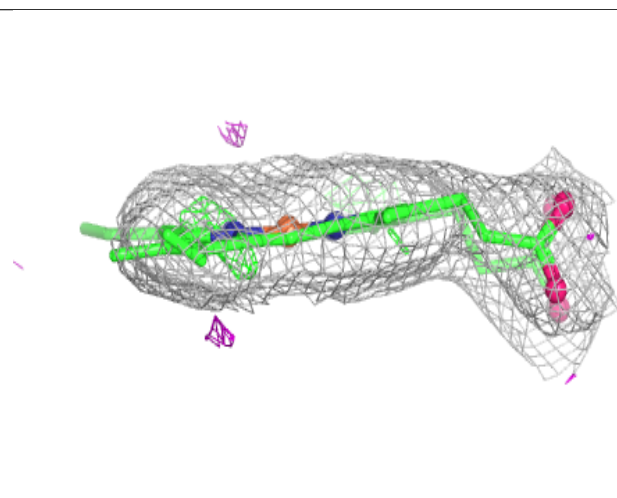
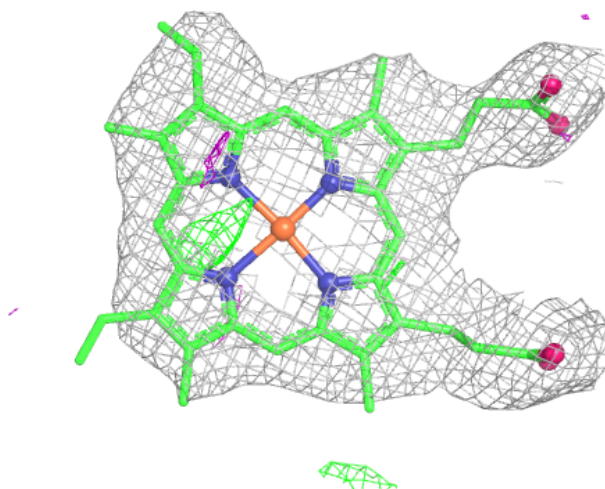
Electron density around 08J B 602:

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



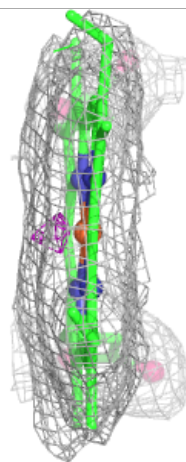
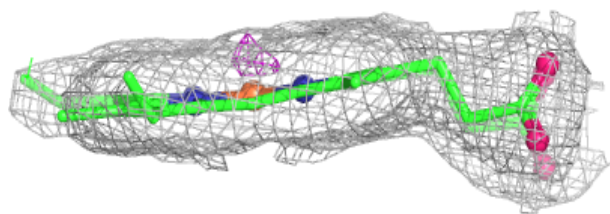
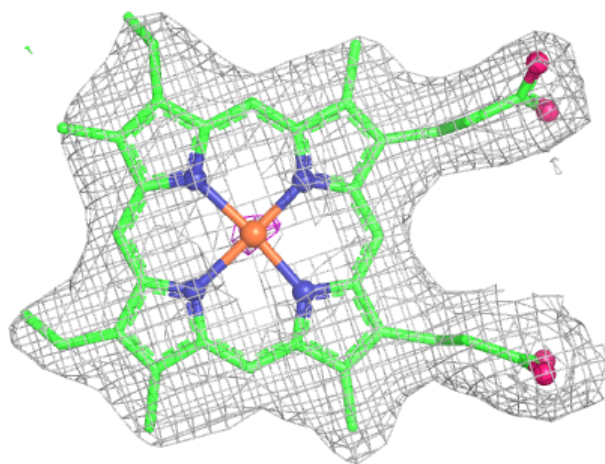
Electron density around HEM C 601:

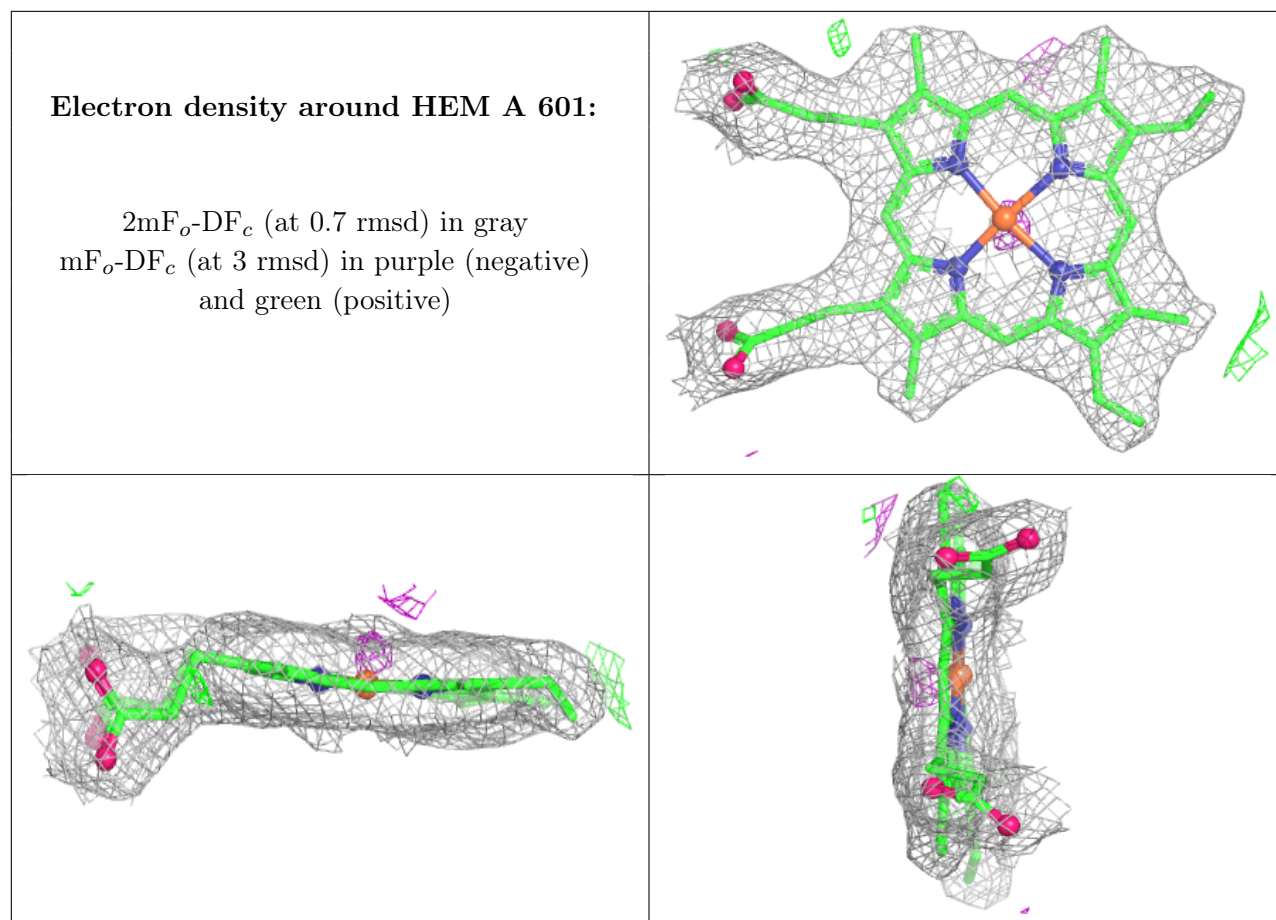
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.