



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 05:59 AM EDT

PDB ID : 3SWZ
Title : Human Cytochrome P450 17A1 in complex with TOK-001
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2011-07-14
Resolution : 2.40 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
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

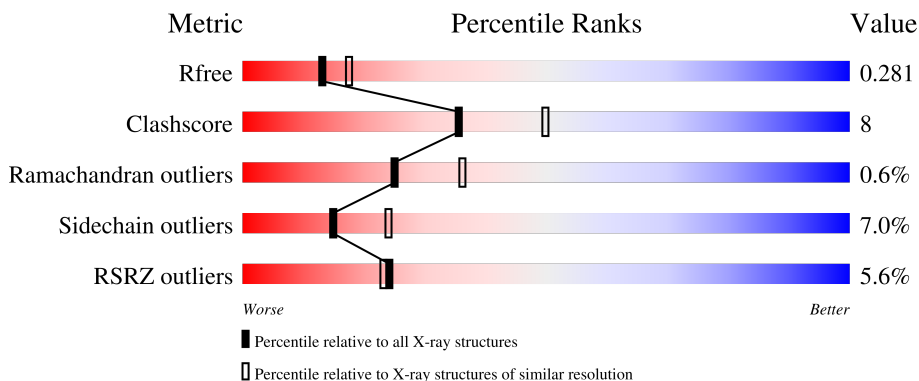
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


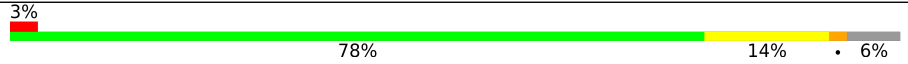
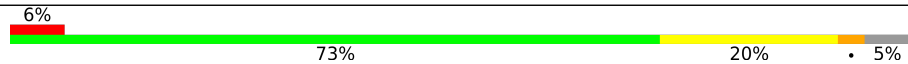

The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	 6% 79% 15% • 5%
1	B	494	 3% 78% 14% • 6%
1	C	494	 6% 73% 20% • 5%
1	D	494	 6% 70% 22% • 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15296 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	3748	2401	649	683	15	0	0	0
1	B	465	3708	2380	641	672	15	0	0	0
1	C	470	3750	2404	649	682	15	0	1	0
1	D	466	3714	2383	642	674	15	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	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	-	expression tag	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	-	expression tag	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	expression tag	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



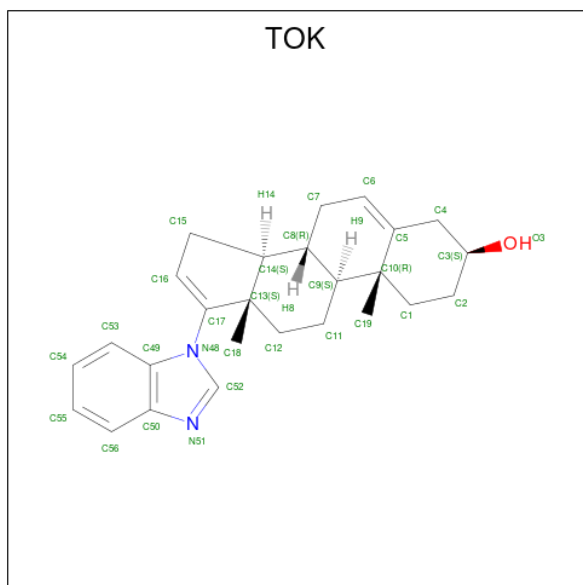
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is (3alpha,8alpha)-17-(1H-benzimidazol-1-yl)androsta-5,16-dien-3-ol (three-letter code: TOK) (formula: C₂₆H₃₂N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	26	2	1	0	0
3	B	1	29	26	2	1	0	0
3	C	1	29	26	2	1	0	0
3	D	1	29	26	2	1	0	0

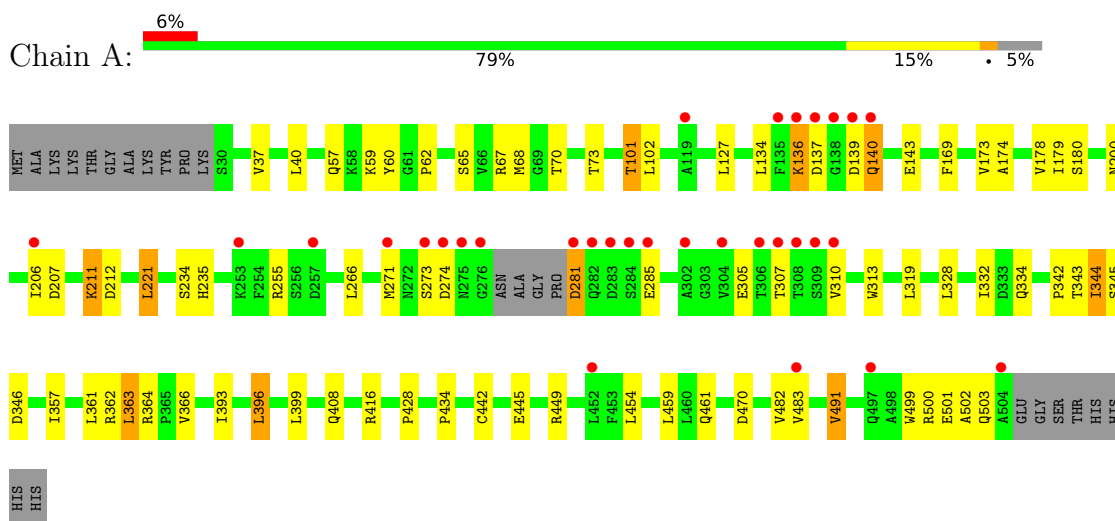
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	23	Total	O	0	0
			23	23		
4	C	22	Total	O	0	0
			22	22		
4	D	17	Total	O	0	0
			17	17		

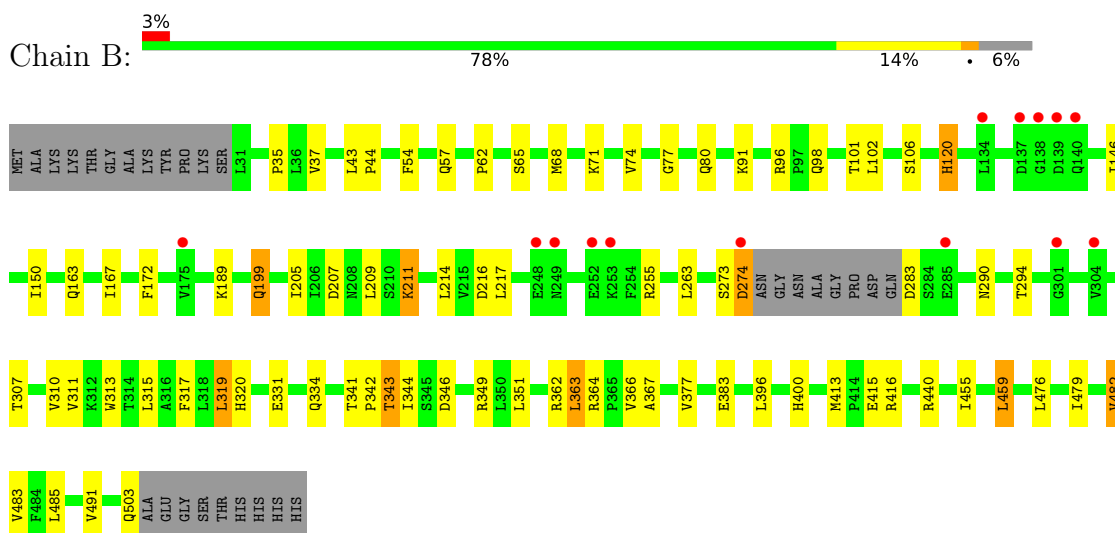
3 Residue-property plots [i](#)

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

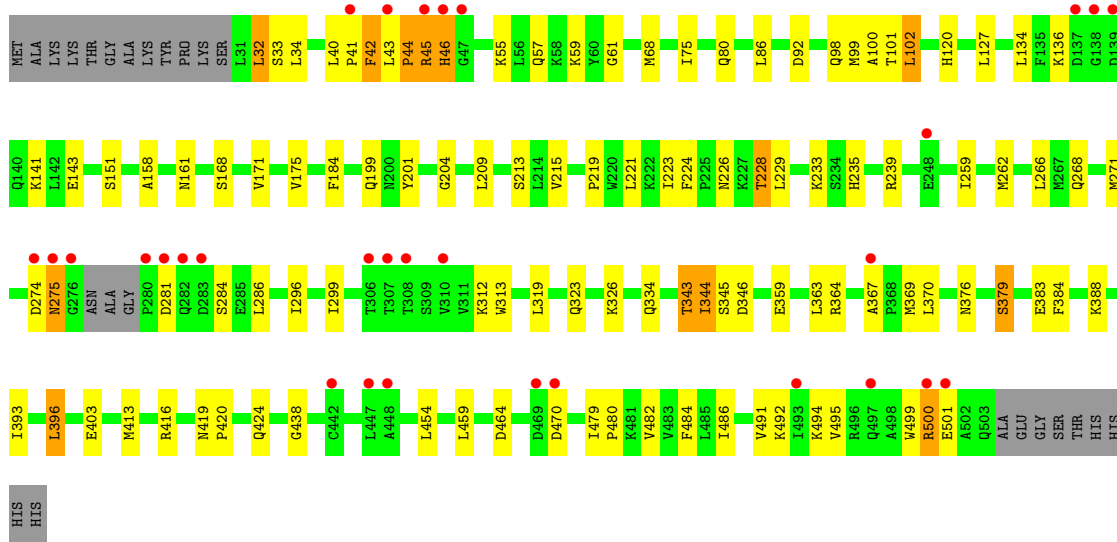


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

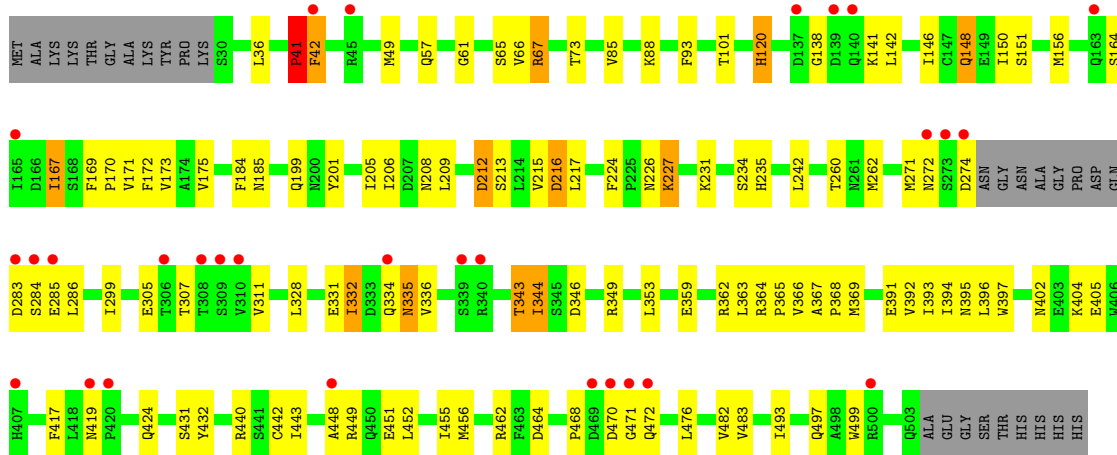


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase





● 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	91.42Å 152.09Å 167.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.08 – 2.40 37.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.08-2.40) 100.0 (37.08-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.223 , 0.288 0.219 , 0.281	Depositor DCC
R_{free} test set	4600 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15296	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: TOK, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	1/3828 (0.0%)	0.78	1/5182 (0.0%)
1	B	0.75	0/3788	0.80	0/5128
1	C	0.79	0/3834	0.84	0/5190
1	D	0.72	0/3794	0.80	4/5136 (0.1%)
All	All	0.75	1/15244 (0.0%)	0.80	5/20636 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASP	C-O	5.55	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	PRO	CA-N-CD	-9.07	98.81	111.50
1	D	440	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	216	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	212	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	491	VAL	CB-CA-C	-5.03	101.84	111.40

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	3748	0	3810	47	0
1	B	3708	0	3779	46	0
1	C	3750	0	3816	68	0
1	D	3714	0	3784	85	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
3	A	29	0	32	3	0
3	B	29	0	32	3	0
3	C	29	0	32	5	0
3	D	29	0	32	2	0
4	A	26	0	0	1	0
4	B	23	0	0	2	0
4	C	22	0	0	2	0
4	D	17	0	0	2	0
All	All	15296	0	15437	247	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 8.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:MET:HB2	1:D:212:ASP:OD2	1.50	1.08
1:D:328:LEU:O	1:D:332:ILE:HG22	1.62	0.99
1:D:167:ILE:HD13	1:D:167:ILE:H	1.29	0.97
1:D:146:ILE:HG22	1:D:150:ILE:HD11	1.46	0.94
1:D:73:THR:HB	1:D:217:LEU:HD21	1.54	0.89
1:D:148:GLN:HA	1:D:148:GLN:HE21	1.40	0.87
1:D:328:LEU:O	1:D:332:ILE:CG2	2.25	0.85
1:C:323:GLN:CG	4:C:15:HOH:O	2.26	0.84
1:C:323:GLN:HG3	4:C:15:HOH:O	1.78	0.81
1:C:41:PRO:HG2	1:C:42:PHE:N	2.01	0.75
1:C:226:ASN:OD1	1:C:228:THR:HG23	1.86	0.75
1:B:319:LEU:HD21	1:B:491:VAL:HG12	1.66	0.75
1:C:209:LEU:HD23	1:C:482:VAL:HG11	1.69	0.73
1:C:101:THR:OG1	1:C:209:LEU:HD12	1.89	0.72
1:B:68:MET:CE	1:C:40:LEU:HD12	2.20	0.72
1:D:402:ASN:HB3	1:D:405:GLU:HB2	1.70	0.71
1:D:497:GLN:HB2	4:D:518:HOH:O	1.91	0.71
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LEU:HD11	1:C:233:LYS:HE3	1.71	0.70
1:A:416:ARG:O	1:A:428:PRO:HG3	1.91	0.69
1:C:41:PRO:HG2	1:C:42:PHE:H	1.58	0.69
1:A:328:LEU:O	1:A:332:ILE:HG22	1.92	0.69
1:D:146:ILE:CG2	1:D:150:ILE:HD11	2.20	0.69
1:D:307:THR:HG21	1:D:451:GLU:OE1	1.93	0.68
1:C:41:PRO:CG	1:C:42:PHE:N	2.56	0.68
1:D:331:GLU:O	1:D:335:ASN:ND2	2.26	0.68
1:D:41:PRO:HD2	1:D:42:PHE:N	2.09	0.68
1:D:146:ILE:HG22	1:D:150:ILE:CD1	2.23	0.68
1:D:49:MET:CB	1:D:212:ASP:OD2	2.37	0.67
1:D:283:ASP:HA	1:D:286:LEU:CD1	2.25	0.66
1:D:167:ILE:H	1:D:167:ILE:CD1	2.07	0.65
1:D:206:ILE:HD11	1:D:305:GLU:HG3	1.78	0.65
1:B:273:SER:OG	1:B:274:ASP:N	2.30	0.64
1:D:146:ILE:O	1:D:150:ILE:HG13	1.97	0.64
1:D:283:ASP:HA	1:D:286:LEU:HD12	1.78	0.64
3:C:601:TOK:H18B	3:C:601:TOK:H53	1.79	0.63
1:D:365:PRO:O	1:D:368:PRO:HD3	1.99	0.62
3:A:601:TOK:H53	3:A:601:TOK:H18B	1.80	0.62
1:C:41:PRO:CG	1:C:42:PHE:H	2.12	0.62
1:D:226:ASN:OD1	1:D:227:LYS:N	2.33	0.62
1:C:43:LEU:O	1:C:44:PRO:O	2.18	0.62
1:D:148:GLN:HA	1:D:148:GLN:NE2	2.14	0.60
1:A:37:VAL:HG22	1:D:65:SER:O	2.02	0.60
1:C:215:VAL:HG13	1:C:393:ILE:CD1	2.32	0.60
1:C:44:PRO:O	1:C:45:ARG:HB3	2.01	0.59
1:D:49:MET:HB2	1:D:212:ASP:CG	2.22	0.59
1:B:106:SER:O	1:B:294:THR:HG21	2.03	0.59
1:C:419:ASN:ND2	1:C:424:GLN:HG2	2.17	0.59
1:A:343:THR:HG22	1:A:345:SER:H	1.68	0.58
1:B:120:HIS:ND1	1:B:120:HIS:N	2.45	0.58
1:D:215:VAL:HG13	1:D:393:ILE:HD11	1.85	0.58
2:D:600:HEM:C1B	3:D:601:TOK:H56	2.39	0.58
1:C:370:LEU:HD21	1:C:396:LEU:HG	1.86	0.58
1:C:75:ILE:HD12	1:C:75:ILE:N	2.20	0.57
1:D:41:PRO:HD2	1:D:42:PHE:H	1.68	0.57
1:C:120:HIS:NE2	1:C:286:LEU:HD22	2.19	0.57
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.86	0.57
1:C:343:THR:O	1:C:346:ASP:HB2	2.05	0.57
1:B:199:GLN:NE2	4:B:526:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:THR:OG1	1:D:209:LEU:HD12	2.04	0.56
1:D:443:ILE:HD11	2:D:600:HEM:HMD2	1.87	0.56
1:A:273:SER:O	1:A:281:ASP:HB3	2.05	0.56
1:A:313:TRP:CZ3	1:A:364:ARG:HG3	2.40	0.56
1:B:211:LYS:HD3	1:B:211:LYS:C	2.26	0.56
1:C:492:LYS:HE2	1:C:494:LYS:HD3	1.86	0.56
1:C:262:MET:SD	1:C:299:ILE:HG13	2.47	0.55
1:C:367:ALA:HB2	3:C:601:TOK:C55	2.36	0.55
1:B:167:ILE:CD1	1:B:315:LEU:HD11	2.36	0.55
1:C:271:MET:HA	1:C:274:ASP:HB2	1.89	0.55
1:C:313:TRP:CE3	1:C:486:ILE:HD12	2.42	0.55
1:A:57:GLN:HG2	1:A:62:PRO:HA	1.88	0.55
1:A:366:VAL:CG1	1:A:483:VAL:HG13	2.36	0.55
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.39	0.55
1:C:209:LEU:HD23	1:C:482:VAL:CG1	2.37	0.55
1:A:134:LEU:O	1:A:140:GLN:NE2	2.39	0.55
1:B:205:ILE:O	1:B:209:LEU:HB2	2.07	0.55
1:C:223:ILE:HG13	1:C:224:PHE:CD2	2.41	0.54
1:D:262:MET:SD	1:D:299:ILE:HG13	2.47	0.54
1:D:216:ASP:OD1	1:D:216:ASP:O	2.26	0.54
1:C:223:ILE:HD12	1:C:224:PHE:CE2	2.43	0.54
1:A:40:LEU:HD21	1:A:68:MET:HE2	1.89	0.54
1:D:65:SER:HA	1:D:73:THR:O	2.08	0.54
1:D:284:SER:C	1:D:286:LEU:H	2.12	0.54
1:D:448:ALA:O	1:D:452:LEU:HG	2.07	0.53
1:B:167:ILE:HD11	1:B:315:LEU:HD11	1.91	0.53
1:B:343:THR:O	1:B:346:ASP:HB2	2.09	0.53
1:B:290:ASN:HB3	4:B:514:HOH:O	2.09	0.53
1:D:57:GLN:O	1:D:61:GLY:N	2.33	0.52
1:B:205:ILE:HG21	3:B:601:TOK:H4A	1.92	0.52
1:D:424:GLN:NE2	4:D:513:HOH:O	2.26	0.52
2:A:600:HEM:C1D	3:A:601:TOK:H52	2.44	0.52
1:A:366:VAL:HG13	1:A:483:VAL:HG13	1.91	0.52
1:A:499:TRP:O	1:A:503:GLN:HG2	2.10	0.52
1:C:171:VAL:O	1:C:175:VAL:HG22	2.11	0.51
1:C:226:ASN:OD1	1:C:228:THR:CG2	2.57	0.51
1:B:311:VAL:O	1:B:315:LEU:HG	2.09	0.51
1:D:493:ILE:HG23	1:D:493:ILE:O	2.11	0.51
1:A:206:ILE:HD11	1:A:305:GLU:HG3	1.92	0.51
1:D:41:PRO:CD	1:D:42:PHE:N	2.74	0.51
1:A:500:ARG:HG3	1:A:500:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:THR:HB	1:B:342:PRO:CD	2.41	0.51
1:C:45:ARG:HG3	1:C:46:HIS:N	2.26	0.51
1:A:235:HIS:HD2	4:A:532:HOH:O	1.92	0.50
1:C:120:HIS:CD2	1:C:286:LEU:HD22	2.46	0.50
1:B:362:ARG:HA	1:B:400:HIS:HD1	1.76	0.50
1:A:67:ARG:HB2	1:D:36:LEU:HD11	1.93	0.50
1:C:274:ASP:O	1:C:275:ASN:O	2.30	0.49
1:D:167:ILE:HD13	1:D:167:ILE:N	2.13	0.49
1:D:138:GLY:H	1:D:141:LYS:HB2	1.76	0.49
1:B:317:PHE:CZ	1:B:363:LEU:HD13	2.48	0.49
1:D:164:SER:HB3	1:D:468:PRO:HB3	1.93	0.49
1:B:274:ASP:OD1	1:B:274:ASP:O	2.30	0.49
1:D:224:PHE:HB2	1:D:226:ASN:HD22	1.77	0.49
1:D:274:ASP:OD1	1:D:274:ASP:O	2.29	0.49
1:D:216:ASP:HB3	1:D:391:GLU:OE1	2.12	0.49
1:D:335:ASN:N	1:D:335:ASN:HD22	2.10	0.49
1:B:68:MET:HE3	1:C:40:LEU:HD12	1.92	0.49
1:C:201:TYR:CE1	1:C:239:ARG:HG2	2.47	0.49
1:D:311:VAL:HG21	1:D:455:ILE:HD13	1.95	0.49
1:C:136:LYS:O	1:C:141:LYS:HG3	2.13	0.48
1:C:359:GLU:HA	1:C:359:GLU:OE1	2.13	0.48
1:B:35:PRO:HD3	1:C:384:PHE:CE2	2.48	0.48
1:D:335:ASN:ND2	1:D:335:ASN:N	2.61	0.48
1:C:495:VAL:HB	1:C:500:ARG:NH1	2.29	0.48
1:D:359:GLU:OE1	1:D:359:GLU:HA	2.14	0.48
1:D:442:CYS:HB2	2:D:600:HEM:C4A	2.48	0.48
1:B:54:PHE:O	1:B:57:GLN:HB2	2.14	0.48
1:A:500:ARG:HG3	1:A:500:ARG:NH1	2.29	0.47
1:A:200:ASN:HB3	1:B:163:GLN:NE2	2.29	0.47
1:B:167:ILE:HD11	1:B:315:LEU:CD1	2.43	0.47
2:A:600:HEM:C1B	3:A:601:TOK:H56	2.49	0.47
1:D:344:ILE:HD13	1:D:344:ILE:HA	1.67	0.47
1:A:442:CYS:HB2	2:A:600:HEM:NA	2.30	0.47
1:D:362:ARG:NH2	1:D:363:LEU:HG	2.29	0.47
1:B:101:THR:HG23	1:B:102:LEU:N	2.30	0.47
1:C:367:ALA:HB2	3:C:601:TOK:H55	1.96	0.47
1:B:366:VAL:HG12	1:B:483:VAL:HG13	1.97	0.47
1:C:313:TRP:CE3	1:C:364:ARG:HG3	2.49	0.47
1:A:101:THR:CG2	1:A:102:LEU:N	2.78	0.46
1:D:142:LEU:O	1:D:146:ILE:HG13	2.16	0.46
1:C:41:PRO:CD	1:C:42:PHE:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ILE:HD12	1:D:336:VAL:HG21	1.97	0.46
1:D:343:THR:O	1:D:346:ASP:HB2	2.15	0.46
1:C:99:MET:O	1:C:100:ALA:C	2.53	0.46
1:C:376:ASN:O	1:C:388:LYS:HE3	2.16	0.46
1:D:205:ILE:O	1:D:209:LEU:HB2	2.15	0.46
1:D:49:MET:HB3	1:D:369:MET:HE1	1.98	0.46
1:A:40:LEU:HD21	1:A:68:MET:CE	2.46	0.45
1:A:140:GLN:H	1:A:140:GLN:HG3	1.64	0.45
1:A:357:ILE:O	1:A:361:LEU:HG	2.15	0.45
1:B:57:GLN:HG2	1:B:62:PRO:HA	1.98	0.45
1:A:501:GLU:C	1:A:503:GLN:H	2.19	0.45
1:C:41:PRO:HG2	1:C:42:PHE:HB2	1.98	0.45
1:C:92:ASP:OD2	1:C:379:SER:OG	2.26	0.45
1:D:215:VAL:HG13	1:D:393:ILE:CD1	2.45	0.45
1:A:73:THR:CG2	1:A:393:ILE:HD12	2.47	0.45
1:A:362:ARG:NH2	1:A:363:LEU:HG	2.32	0.45
1:B:362:ARG:HA	1:B:400:HIS:ND1	2.32	0.45
1:C:86:LEU:O	1:C:438:GLY:HA3	2.17	0.45
1:D:242:LEU:HD23	1:D:242:LEU:C	2.37	0.45
1:A:211:LYS:HD3	1:A:211:LYS:C	2.37	0.44
1:A:127:LEU:HD13	1:A:266:LEU:HD23	1.99	0.44
1:B:65:SER:HB3	1:B:74:VAL:HG22	1.98	0.44
1:C:313:TRP:CZ3	1:C:364:ARG:HG3	2.52	0.44
1:D:85:VAL:HG11	1:D:394:ILE:HD11	1.99	0.44
1:D:364:ARG:HH21	1:D:476:LEU:HB3	1.82	0.44
1:C:158:ALA:O	1:C:161:ASN:CB	2.66	0.44
1:D:462:ARG:HA	1:D:499:TRP:CD1	2.53	0.44
1:A:59:LYS:HE3	1:A:60:TYR:CZ	2.53	0.43
1:D:120:HIS:CD2	1:D:120:HIS:H	2.35	0.43
1:A:221:LEU:HD12	1:A:221:LEU:C	2.38	0.43
1:B:263:LEU:HD12	1:B:263:LEU:HA	1.85	0.43
1:A:310:VAL:HG21	2:A:600:HEM:CBB	2.48	0.43
1:D:169:PHE:O	1:D:173:VAL:HG23	2.18	0.43
1:D:367:ALA:HA	1:D:368:PRO:HD2	1.85	0.43
1:A:136:LYS:O	1:A:137:ASP:HB3	2.18	0.43
1:D:353:LEU:HD11	1:D:456:MET:HB3	1.99	0.43
1:D:362:ARG:HB2	1:D:432:TYR:HE1	1.83	0.43
2:B:600:HEM:C1B	3:B:601:TOK:H56	2.54	0.43
1:C:57:GLN:HG2	1:C:61:GLY:O	2.18	0.43
1:C:259:ILE:HG13	1:C:268:GLN:NE2	2.33	0.43
1:B:455:ILE:CG2	1:B:459:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ILE:HG12	1:C:454:LEU:HD11	2.00	0.43
1:D:359:GLU:HA	1:D:417:PHE:HE1	1.83	0.43
1:A:37:VAL:CG2	1:D:66:VAL:HG22	2.49	0.43
1:B:62:PRO:O	1:B:77:GLY:N	2.32	0.43
2:C:600:HEM:C1D	3:C:601:TOK:H52	2.53	0.43
1:A:174:ALA:O	1:A:178:VAL:HG23	2.19	0.43
1:B:413:MET:O	1:B:416:ARG:HG2	2.19	0.42
1:C:127:LEU:HD13	1:C:266:LEU:HD23	2.01	0.42
1:D:67:ARG:HE	1:D:67:ARG:HB3	1.68	0.42
1:A:396:LEU:HD11	1:A:434:PRO:HA	2.00	0.42
1:C:184:PHE:CZ	1:C:296:ILE:HG21	2.54	0.42
1:A:179:ILE:HD12	1:A:179:ILE:HA	1.95	0.42
1:B:313:TRP:CZ3	1:B:364:ARG:HG3	2.55	0.42
1:C:34:LEU:HD12	1:C:34:LEU:C	2.40	0.42
1:D:470:ASP:O	1:D:472:GLN:N	2.52	0.42
1:B:383:GLU:O	1:C:32:LEU:HB2	2.18	0.42
1:D:205:ILE:HG13	1:D:235:HIS:HB3	2.02	0.42
1:D:395:ASN:OD1	1:D:397:TRP:HB3	2.20	0.42
1:C:419:ASN:HB2	1:C:420:PRO:HD2	2.01	0.42
1:D:366:VAL:HG21	2:D:600:HEM:HBB2	2.02	0.42
1:C:479:ILE:HA	1:C:480:PRO:HD3	1.88	0.42
1:A:143:GLU:OE2	1:A:343:THR:HG23	2.20	0.42
1:C:343:THR:HG23	1:C:345:SER:H	1.85	0.42
1:B:96:ARG:HG2	1:B:440:ARG:NH2	2.35	0.42
1:B:214:LEU:HD11	1:B:482:VAL:HG12	2.01	0.42
1:D:206:ILE:CD1	1:D:305:GLU:HG3	2.46	0.42
1:B:146:ILE:O	1:B:150:ILE:HG13	2.20	0.41
1:C:101:THR:HG23	1:C:102:LEU:HD13	2.02	0.41
1:C:204:GLY:HA3	1:C:235:HIS:CE1	2.55	0.41
1:D:283:ASP:HA	1:D:286:LEU:HD13	2.01	0.41
1:B:331:GLU:OE2	1:B:351:LEU:N	2.54	0.41
1:C:219:PRO:O	1:C:223:ILE:HG23	2.21	0.41
1:C:344:ILE:HD13	1:C:344:ILE:HA	1.92	0.41
1:B:214:LEU:HD11	1:B:482:VAL:CG1	2.49	0.41
1:C:158:ALA:O	1:C:161:ASN:HB2	2.20	0.41
1:A:101:THR:HG23	1:A:102:LEU:N	2.35	0.41
1:C:213:SER:HB2	1:C:369:MET:HE3	2.03	0.41
1:D:184:PHE:O	1:D:185:ASN:HB2	2.21	0.41
1:D:185:ASN:OD1	1:D:260:THR:OG1	2.39	0.41
1:A:221:LEU:HD12	1:A:221:LEU:O	2.21	0.41
1:A:169:PHE:O	1:A:173:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:TRP:CZ3	1:C:486:ILE:HD12	2.55	0.41
1:D:41:PRO:CD	1:D:42:PHE:H	2.32	0.41
1:D:167:ILE:CD1	1:D:167:ILE:N	2.81	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.95	0.41
1:A:65:SER:HA	1:A:73:THR:O	2.21	0.41
1:A:344:ILE:HD13	1:A:344:ILE:HA	1.69	0.41
1:B:479:ILE:N	1:B:485:LEU:O	2.51	0.41
1:A:343:THR:O	1:A:346:ASP:HB2	2.21	0.41
1:B:37:VAL:O	1:C:41:PRO:HD3	2.20	0.41
1:B:310:VAL:HG22	1:B:366:VAL:HG22	2.03	0.41
1:C:168:SER:OG	1:C:312:LYS:HD2	2.21	0.41
1:D:93:PHE:CD1	1:D:392:VAL:HG21	2.56	0.41
1:A:342:PRO:HD3	1:A:461:GLN:OE1	2.21	0.40
1:B:43:LEU:HA	1:B:44:PRO:HD3	1.82	0.40
1:B:320:HIS:CD2	1:B:476:LEU:HD11	2.57	0.40
1:D:208:ASN:OD1	1:D:231:LYS:HE3	2.20	0.40
1:C:482:VAL:O	3:C:601:TOK:H54	2.21	0.40
1:D:212:ASP:CG	1:D:213:SER:H	2.25	0.40
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.87	0.40
3:D:601:TOK:H19B	3:D:601:TOK:H11	1.89	0.40
1:B:189:LYS:HD3	1:B:189:LYS:HA	1.95	0.40
1:B:367:ALA:HB2	3:B:601:TOK:C55	2.51	0.40
1:D:171:VAL:O	1:D:175:VAL:HG22	2.21	0.40
1:D:366:VAL:CG1	1:D:483:VAL:HG13	2.52	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	467/494 (94%)	443 (95%)	23 (5%)	1 (0%)	47 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	461/494 (93%)	434 (94%)	27 (6%)	0	100	100
1	C	467/494 (94%)	433 (93%)	28 (6%)	6 (1%)	12	17
1	D	462/494 (94%)	414 (90%)	43 (9%)	5 (1%)	14	20
All	All	1857/1976 (94%)	1724 (93%)	121 (6%)	12 (1%)	25	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	ARG
1	C	275	ASN
1	D	41	PRO
1	A	502	ALA
1	C	46	HIS
1	D	272	ASN
1	D	471	GLY
1	D	404	LYS
1	C	44	PRO
1	D	285	GLU
1	C	284	SER
1	C	134	LEU

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	419/436 (96%)	392 (94%)	27 (6%)	17	28
1	B	415/436 (95%)	388 (94%)	27 (6%)	17	27
1	C	420/436 (96%)	384 (91%)	36 (9%)	10	16
1	D	416/436 (95%)	389 (94%)	27 (6%)	17	27
All	All	1670/1744 (96%)	1553 (93%)	117 (7%)	15	24

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	101	THR
1	A	136	LYS
1	A	139	ASP
1	A	140	GLN
1	A	180	SER
1	A	207	ASP
1	A	211	LYS
1	A	221	LEU
1	A	234	SER
1	A	255	ARG
1	A	271	MET
1	A	274	ASP
1	A	281	ASP
1	A	285	GLU
1	A	307	THR
1	A	319	LEU
1	A	334	GLN
1	A	344	ILE
1	A	363	LEU
1	A	396	LEU
1	A	399	LEU
1	A	408	GLN
1	A	459	LEU
1	A	470	ASP
1	A	482	VAL
1	A	491	VAL
1	B	71	LYS
1	B	80	GLN
1	B	91	LYS
1	B	98	GLN
1	B	120	HIS
1	B	172	PHE
1	B	199	GLN
1	B	207	ASP
1	B	211	LYS
1	B	216	ASP
1	B	217	LEU
1	B	255	ARG
1	B	274	ASP
1	B	283	ASP
1	B	307	THR
1	B	319	LEU

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Mol	Chain	Res	Type
1	B	334	GLN
1	B	343	THR
1	B	344	ILE
1	B	349	ARG
1	B	363	LEU
1	B	377	VAL
1	B	396	LEU
1	B	415	GLU
1	B	459	LEU
1	B	482	VAL
1	B	503	GLN
1	C	32	LEU
1	C	33	SER
1	C	42	PHE
1	C	55	LYS
1	C	59	LYS
1	C	68	MET
1	C	80	GLN
1	C	98	GLN
1	C	102	LEU
1	C	143	GLU
1	C	151	SER
1	C	199	GLN
1	C	221	LEU
1	C	228	THR
1	C	281	ASP
1	C	319	LEU
1	C	326	LYS
1	C	334[A]	GLN
1	C	334[B]	GLN
1	C	343	THR
1	C	344	ILE
1	C	363	LEU
1	C	379	SER
1	C	383	GLU
1	C	396	LEU
1	C	403	GLU
1	C	413	MET
1	C	416	ARG
1	C	459	LEU
1	C	464	ASP
1	C	470	ASP

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Mol	Chain	Res	Type
1	C	484	PHE
1	C	491	VAL
1	C	499	TRP
1	C	500	ARG
1	C	501	GLU
1	D	42	PHE
1	D	67	ARG
1	D	88	LYS
1	D	120	HIS
1	D	148	GLN
1	D	151	SER
1	D	156	MET
1	D	167	ILE
1	D	170	PRO
1	D	172	PHE
1	D	199	GLN
1	D	201	TYR
1	D	227	LYS
1	D	234	SER
1	D	271	MET
1	D	332	ILE
1	D	334	GLN
1	D	335	ASN
1	D	343	THR
1	D	344	ILE
1	D	349	ARG
1	D	396	LEU
1	D	419	ASN
1	D	431	SER
1	D	449	ARG
1	D	464	ASP
1	D	482	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	275	ASN
1	A	321	ASN
1	B	140	GLN
1	B	199	GLN
1	B	424	GLN

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Mol	Chain	Res	Type
1	C	268	GLN
1	C	275	ASN
1	C	472	GLN
1	C	503	GLN
1	D	48	HIS
1	D	148	GLN
1	D	335	ASN

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	600	1,3	41,50,50	2.12	10 (24%)	45,82,82	1.94	12 (26%)
2	HEM	B	600	1,3	41,50,50	1.87	7 (17%)	45,82,82	1.91	13 (28%)
3	TOK	D	601	2	34,34,34	1.35	5 (14%)	44,54,54	1.20	6 (13%)
2	HEM	A	600	1,3	41,50,50	2.05	8 (19%)	45,82,82	1.93	12 (26%)
2	HEM	D	600	1,3	41,50,50	2.10	10 (24%)	45,82,82	1.53	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TOK	B	601	2	34,34,34	1.50	6 (17%)	44,54,54	1.50	8 (18%)
3	TOK	C	601	2	34,34,34	1.41	4 (11%)	44,54,54	1.84	13 (29%)
3	TOK	A	601	2	34,34,34	1.33	4 (11%)	44,54,54	1.61	10 (22%)

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	C	600	1,3	-	1/12/54/54	-
2	HEM	B	600	1,3	-	3/12/54/54	-
3	TOK	D	601	2	-	0/0/62/62	0/6/6/6
2	HEM	A	600	1,3	-	2/12/54/54	-
2	HEM	D	600	1,3	-	8/12/54/54	-
3	TOK	B	601	2	-	0/0/62/62	0/6/6/6
3	TOK	C	601	2	-	0/0/62/62	0/6/6/6
3	TOK	A	601	2	-	0/0/62/62	0/6/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3D-C2D	7.90	1.53	1.36
2	C	600	HEM	C3D-C2D	7.85	1.53	1.36
2	D	600	HEM	C3D-C2D	7.30	1.52	1.36
2	B	600	HEM	C3D-C2D	6.67	1.50	1.36
2	C	600	HEM	C3C-C2C	-5.39	1.32	1.40
2	D	600	HEM	C3C-C2C	-5.22	1.33	1.40
3	C	601	TOK	C49-N48	-4.90	1.32	1.39
2	B	600	HEM	C3C-C2C	-4.65	1.33	1.40
2	A	600	HEM	C3C-CAC	4.37	1.56	1.47
3	B	601	TOK	C52-N48	-4.35	1.31	1.36
3	D	601	TOK	C52-N48	-4.17	1.32	1.36
3	B	601	TOK	C17-N48	-4.16	1.39	1.46
2	A	600	HEM	C3C-C2C	-3.98	1.34	1.40
3	A	601	TOK	C17-N48	-3.87	1.40	1.46
2	C	600	HEM	CAA-C2A	3.67	1.57	1.52
2	D	600	HEM	C3C-CAC	3.48	1.54	1.47
2	A	600	HEM	CAA-C2A	3.47	1.57	1.52
2	D	600	HEM	CAB-C3B	3.44	1.56	1.47
2	C	600	HEM	C3C-CAC	3.36	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	TOK	C17-N48	-3.34	1.41	1.46
3	D	601	TOK	C16-C17	3.32	1.35	1.32
2	A	600	HEM	CAB-C3B	3.25	1.56	1.47
2	D	600	HEM	C1B-NB	-3.22	1.34	1.40
3	A	601	TOK	C52-N48	-3.22	1.33	1.36
2	A	600	HEM	FE-ND	3.02	2.11	1.96
2	B	600	HEM	C3C-CAC	2.99	1.53	1.47
2	D	600	HEM	CMD-C2D	2.86	1.56	1.50
2	C	600	HEM	FE-NB	2.84	2.10	1.96
2	C	600	HEM	FE-ND	2.81	2.10	1.96
3	A	601	TOK	C16-C17	2.80	1.34	1.32
2	D	600	HEM	CAA-C2A	2.76	1.56	1.52
2	B	600	HEM	CAB-C3B	2.72	1.54	1.47
3	B	601	TOK	C54-C53	2.70	1.42	1.36
2	B	600	HEM	FE-ND	2.62	2.09	1.96
3	D	601	TOK	C17-N48	-2.52	1.42	1.46
2	A	600	HEM	CHC-C4B	-2.43	1.34	1.41
2	C	600	HEM	CAB-C3B	2.43	1.54	1.47
3	B	601	TOK	C49-N48	-2.35	1.36	1.39
3	B	601	TOK	C16-C17	2.33	1.34	1.32
3	D	601	TOK	C49-N48	-2.32	1.36	1.39
2	C	600	HEM	CMB-C2B	2.27	1.55	1.50
3	B	601	TOK	C15-C16	2.22	1.53	1.50
3	A	601	TOK	C49-N48	-2.21	1.36	1.39
2	B	600	HEM	CMB-C2B	2.18	1.55	1.50
2	D	600	HEM	CMB-C2B	2.15	1.55	1.50
2	D	600	HEM	C4D-ND	-2.13	1.36	1.40
2	B	600	HEM	CAA-C2A	2.10	1.55	1.52
3	D	601	TOK	C54-C53	2.09	1.41	1.36
2	A	600	HEM	C1B-NB	-2.07	1.36	1.40
2	C	600	HEM	CMD-C2D	2.06	1.55	1.50
2	D	600	HEM	O2D-CGD	-2.03	1.23	1.30
3	C	601	TOK	C52-N48	-2.03	1.34	1.36
3	C	601	TOK	C54-C53	2.03	1.41	1.36
2	C	600	HEM	C4A-NA	2.01	1.40	1.36

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	C4D-ND-C1D	7.05	112.36	105.07
2	B	600	HEM	C4D-ND-C1D	6.48	111.77	105.07
2	A	600	HEM	C4D-ND-C1D	6.32	111.60	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	TOK	C3-C4-C5	-5.66	102.42	112.03
2	D	600	HEM	C4D-ND-C1D	4.67	109.90	105.07
2	A	600	HEM	CMA-C3A-C4A	-4.63	121.35	128.46
3	C	601	TOK	C7-C8-C9	4.43	115.08	109.71
2	C	600	HEM	C4B-CHC-C1C	4.25	128.17	122.56
3	A	601	TOK	C15-C14-C13	3.88	106.95	104.05
3	B	601	TOK	C1-C2-C3	3.87	115.43	110.47
3	B	601	TOK	C15-C14-C13	-3.68	101.29	104.05
2	D	600	HEM	C3B-C2B-C1B	3.65	109.19	106.49
2	B	600	HEM	C2C-C3C-C4C	3.59	109.40	106.90
3	C	601	TOK	C7-C8-C14	3.51	115.99	110.91
2	B	600	HEM	C4C-CHD-C1D	3.50	127.18	122.56
3	A	601	TOK	C14-C8-C9	-3.49	104.42	109.09
2	D	600	HEM	CBA-CAA-C2A	3.43	118.47	112.62
2	C	600	HEM	CMA-C3A-C4A	-3.36	123.30	128.46
2	B	600	HEM	CAA-CBA-CGA	-3.27	104.59	113.76
2	C	600	HEM	C4C-CHD-C1D	3.25	126.84	122.56
2	A	600	HEM	CMA-C3A-C2A	3.22	131.01	124.94
3	B	601	TOK	C3-C4-C5	-3.14	106.69	112.03
2	A	600	HEM	C4C-CHD-C1D	3.11	126.67	122.56
2	C	600	HEM	C1B-NB-C4B	3.10	108.28	105.07
3	C	601	TOK	C19-C10-C1	3.05	114.25	109.43
2	D	600	HEM	C1D-C2D-C3D	-3.02	103.78	106.96
3	C	601	TOK	C1-C2-C3	-3.02	106.59	110.47
2	A	600	HEM	C4B-CHC-C1C	3.01	126.54	122.56
2	A	600	HEM	O2A-CGA-CBA	3.01	123.70	114.03
3	A	601	TOK	C3-C4-C5	-2.97	106.98	112.03
3	A	601	TOK	C12-C11-C9	2.96	118.25	113.11
2	B	600	HEM	CAD-C3D-C4D	2.92	129.75	124.66
2	C	600	HEM	C3B-C2B-C1B	2.90	108.64	106.49
3	D	601	TOK	C4-C5-C6	-2.88	116.45	120.61
2	A	600	HEM	CBA-CAA-C2A	2.82	117.43	112.62
3	D	601	TOK	C15-C14-C13	2.75	106.11	104.05
2	A	600	HEM	O1A-CGA-CBA	-2.70	114.40	123.08
3	A	601	TOK	C12-C13-C17	-2.68	116.39	119.95
2	D	600	HEM	CMD-C2D-C1D	2.64	129.06	125.04
3	C	601	TOK	C4-C5-C10	2.64	119.93	116.42
3	C	601	TOK	C12-C13-C14	-2.64	104.82	108.99
3	A	601	TOK	C19-C10-C1	2.61	113.56	109.43
2	B	600	HEM	CMA-C3A-C4A	-2.61	124.46	128.46
2	D	600	HEM	O2A-CGA-CBA	2.60	122.39	114.03
3	D	601	TOK	C18-C13-C12	-2.56	108.11	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	C3D-C4D-ND	-2.52	107.36	110.17
2	A	600	HEM	CAD-C3D-C4D	2.48	129.00	124.66
2	B	600	HEM	CHD-C1D-ND	2.47	127.11	124.43
3	B	601	TOK	C2-C1-C10	2.46	118.07	112.74
3	C	601	TOK	C19-C10-C9	-2.40	108.82	111.68
3	A	601	TOK	C7-C8-C14	2.39	114.38	110.91
3	B	601	TOK	C18-C13-C14	-2.35	109.51	112.98
3	C	601	TOK	C4-C5-C6	-2.32	117.26	120.61
2	A	600	HEM	C4D-C3D-C2D	-2.31	103.54	106.90
3	C	601	TOK	C18-C13-C14	2.29	116.37	112.98
2	A	600	HEM	CMB-C2B-C1B	-2.29	121.56	125.04
2	B	600	HEM	CAD-CBD-CGD	-2.28	108.69	113.60
3	D	601	TOK	C3-C4-C5	-2.27	108.17	112.03
2	B	600	HEM	O2A-CGA-CBA	2.26	121.28	114.03
2	B	600	HEM	CMA-C3A-C2A	2.22	129.13	124.94
2	C	600	HEM	CAD-CBD-CGD	-2.22	108.82	113.60
3	D	601	TOK	C4-C5-C10	2.21	119.36	116.42
3	C	601	TOK	C9-C10-C5	2.21	113.11	109.65
3	A	601	TOK	C11-C9-C8	2.21	114.94	111.75
2	B	600	HEM	CMD-C2D-C1D	2.21	128.40	125.04
3	B	601	TOK	C7-C8-C14	2.18	114.06	110.91
2	C	600	HEM	CHA-C4D-ND	2.18	127.07	124.38
3	A	601	TOK	C1-C10-C9	-2.15	105.72	108.73
2	B	600	HEM	CAD-C3D-C2D	-2.12	123.92	127.88
3	A	601	TOK	C1-C2-C3	2.12	113.19	110.47
2	A	600	HEM	CMD-C2D-C1D	2.10	128.24	125.04
3	C	601	TOK	C19-C10-C5	-2.07	104.99	108.34
3	B	601	TOK	C19-C10-C9	-2.07	109.22	111.68
2	C	600	HEM	C2B-C1B-NB	-2.07	107.39	109.84
2	B	600	HEM	C3D-C4D-ND	-2.06	107.87	110.17
3	B	601	TOK	C19-C10-C1	2.04	112.65	109.43
2	C	600	HEM	CMD-C2D-C1D	2.03	128.13	125.04
3	C	601	TOK	C14-C8-C9	-2.03	106.38	109.09
2	D	600	HEM	O1A-CGA-CBA	-2.02	116.59	123.08
3	D	601	TOK	C14-C13-C17	-2.01	97.08	100.28
2	C	600	HEM	CMA-C3A-C2A	2.00	128.71	124.94

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	600	HEM	C1A-C2A-CAA-CBA

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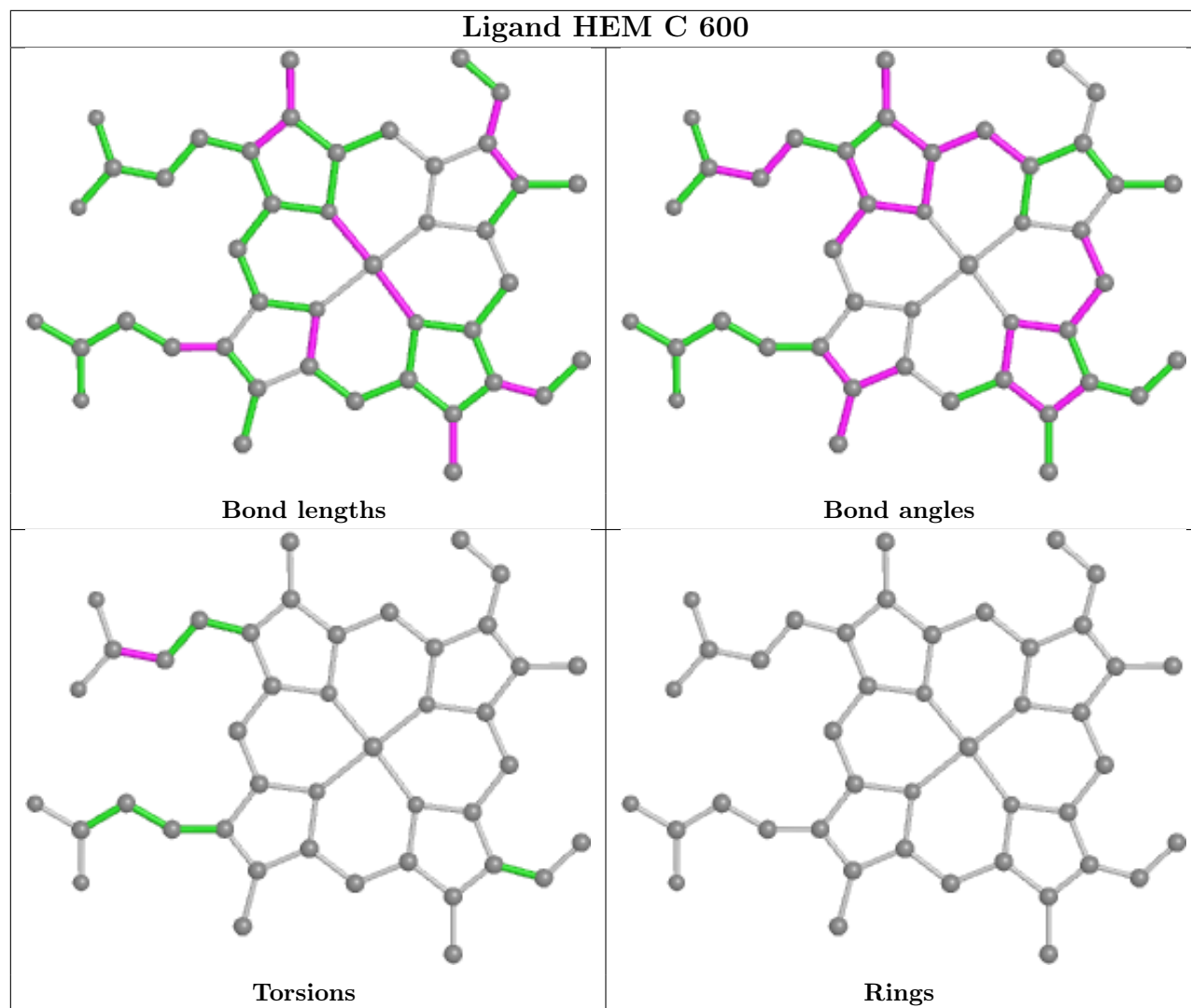
Mol	Chain	Res	Type	Atoms
2	D	600	HEM	C2B-C3B-CAB-CBB
2	D	600	HEM	C4B-C3B-CAB-CBB
2	A	600	HEM	C1A-C2A-CAA-CBA
2	D	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAD-CBD-CGD-O1D
2	B	600	HEM	CAA-CBA-CGA-O2A
2	D	600	HEM	CAD-CBD-CGD-O2D
2	D	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAD-CBD-CGD-O2D
2	C	600	HEM	CAD-CBD-CGD-O2D
2	A	600	HEM	CAD-CBD-CGD-O1D

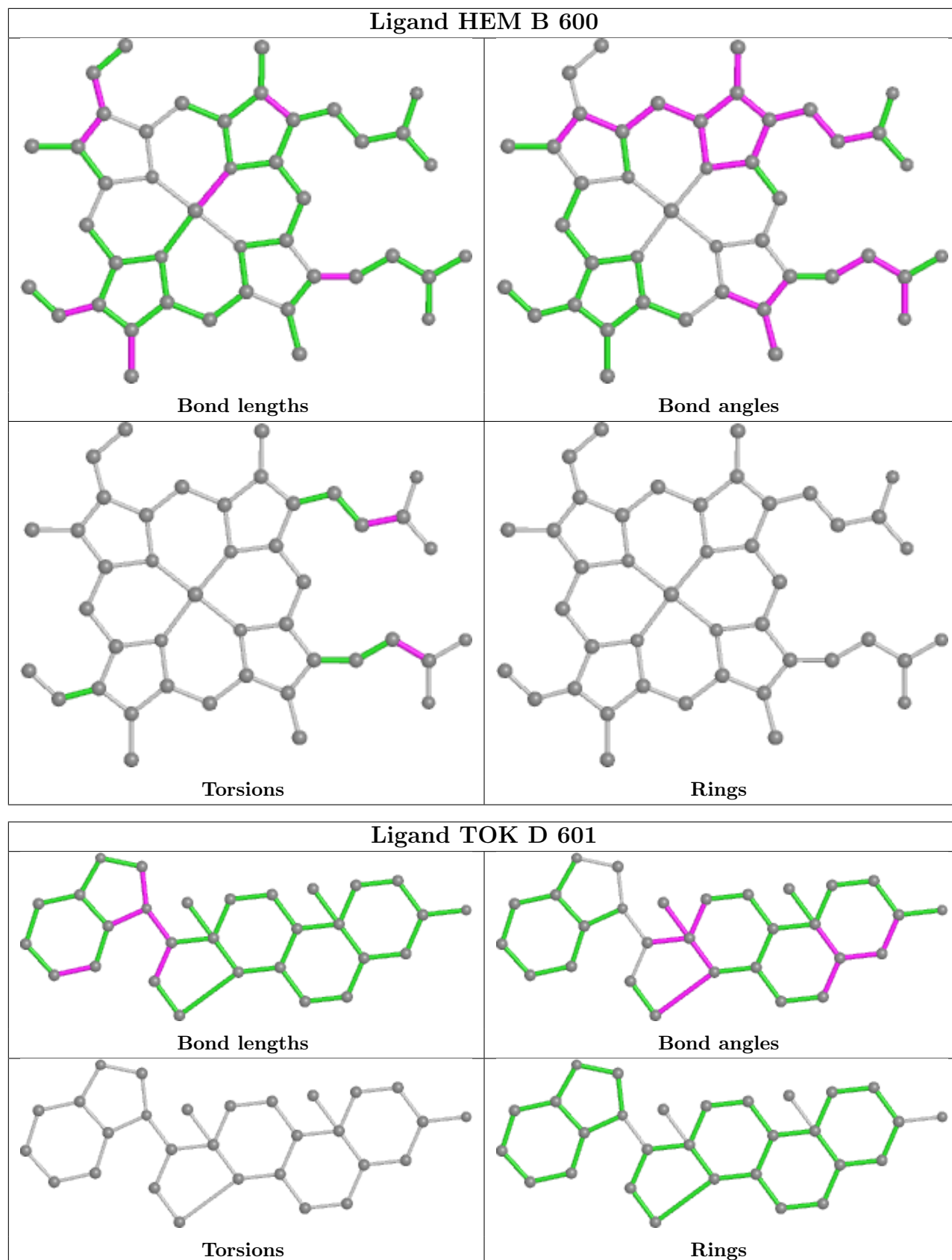
There are no ring outliers.

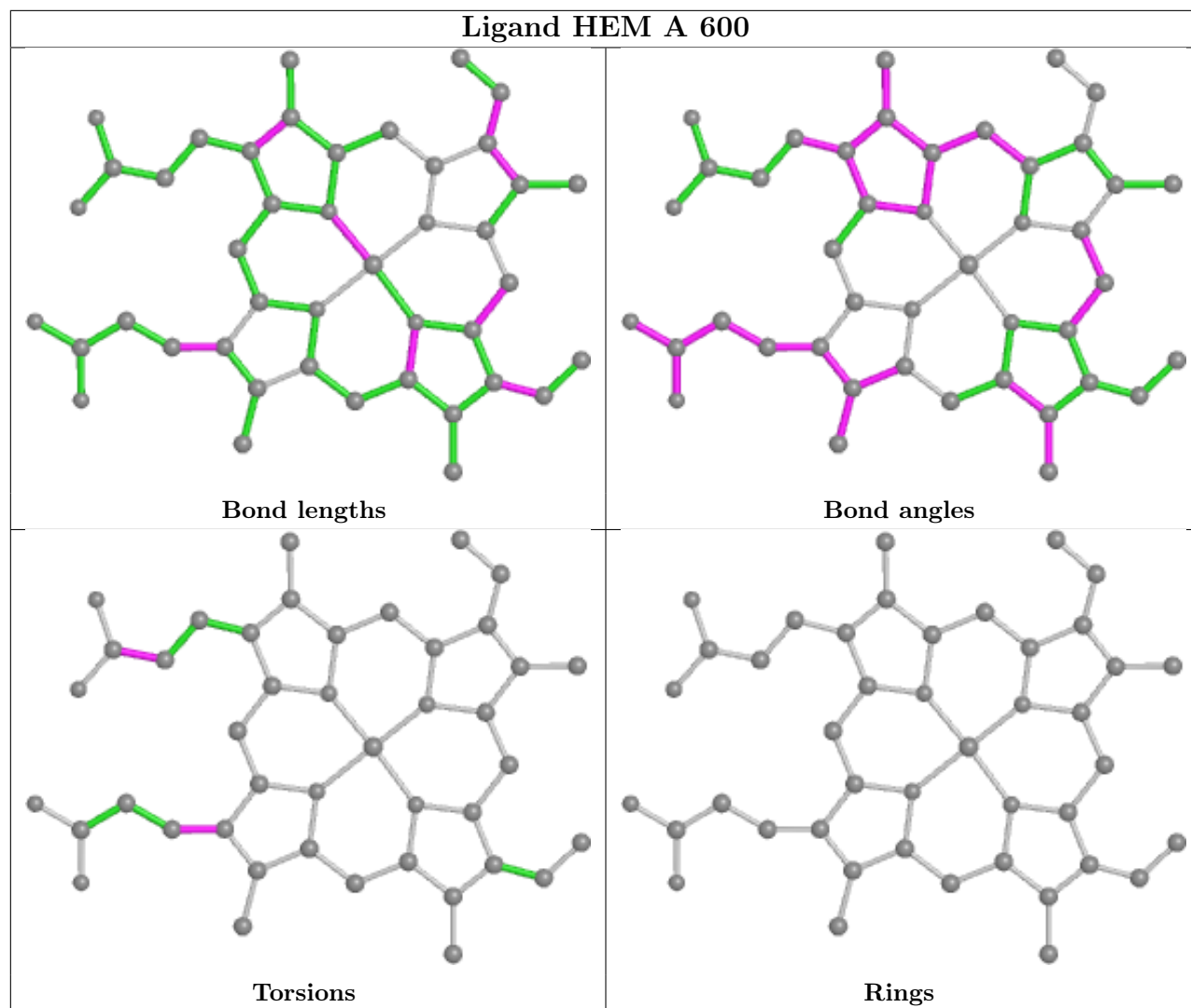
8 monomers are involved in 20 short contacts:

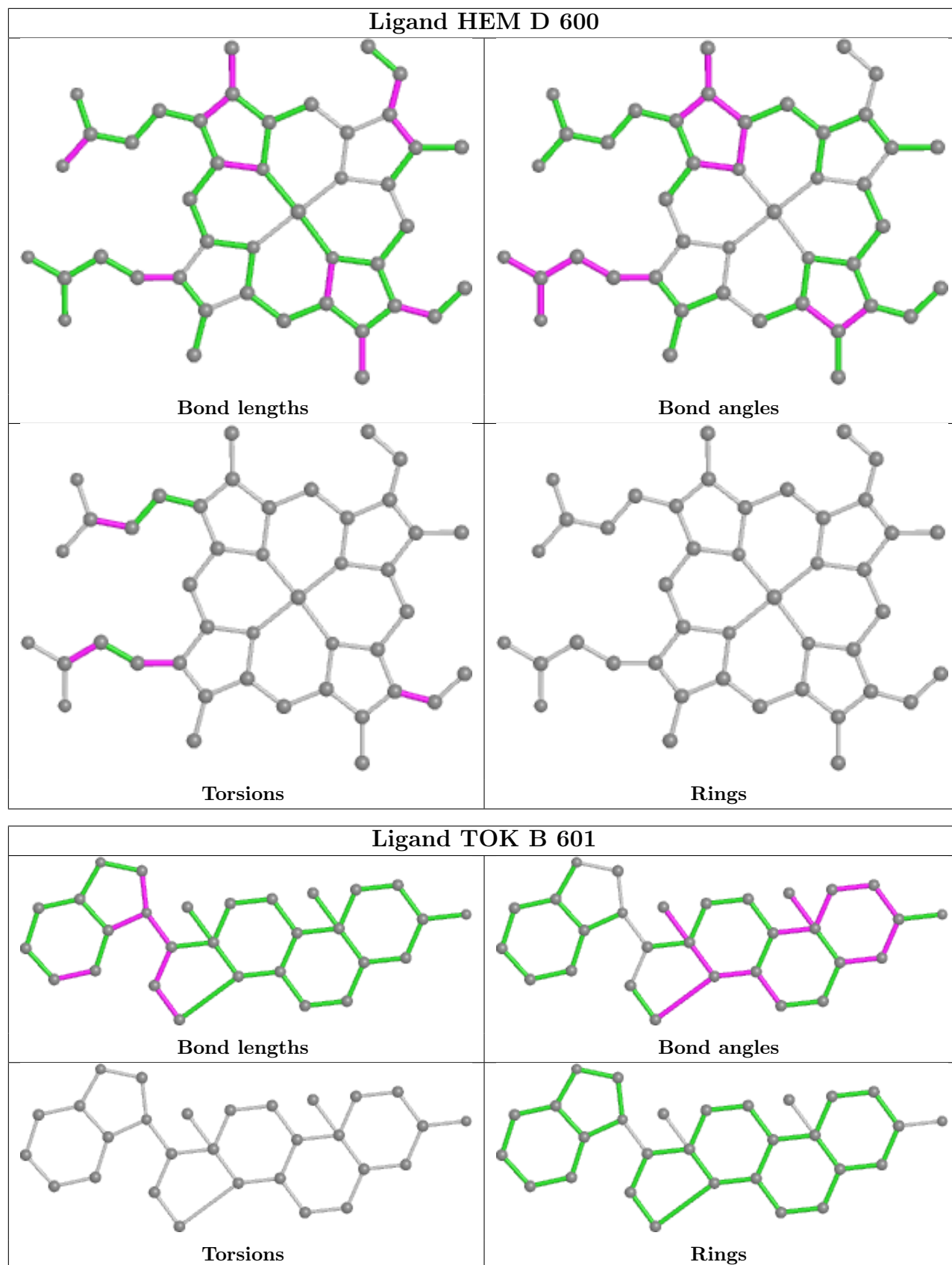
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	HEM	2	0
2	B	600	HEM	1	0
3	D	601	TOK	2	0
2	A	600	HEM	4	0
2	D	600	HEM	5	0
3	B	601	TOK	3	0
3	C	601	TOK	5	0
3	A	601	TOK	3	0

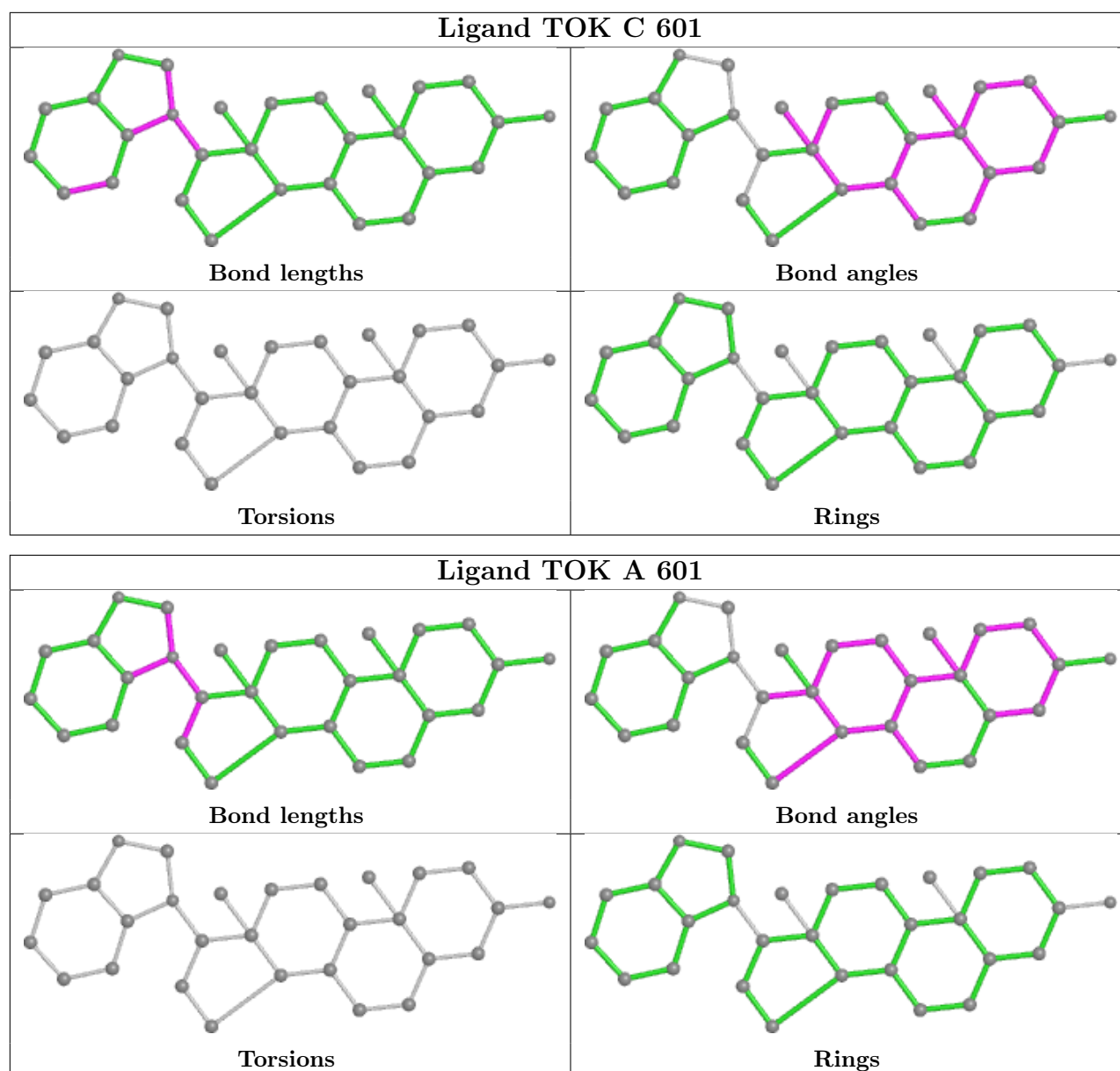
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	471/494 (95%)	0.21	31 (6%) 18 17	29, 44, 70, 81	0
1	B	465/494 (94%)	0.02	14 (3%) 50 49	25, 43, 67, 75	0
1	C	470/494 (95%)	0.21	30 (6%) 19 18	29, 43, 69, 82	0
1	D	466/494 (94%)	0.32	29 (6%) 20 19	27, 48, 75, 87	0
All	All	1872/1976 (94%)	0.19	104 (5%) 24 23	25, 44, 71, 87	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	HIS	6.5
1	C	275	ASN	6.5
1	A	139	ASP	6.2
1	A	282	GLN	5.5
1	B	138	GLY	4.7
1	C	45	ARG	4.6
1	D	469	ASP	4.5
1	A	283	ASP	4.5
1	A	275	ASN	4.5
1	A	135	PHE	4.4
1	C	138	GLY	4.3
1	C	281	ASP	4.3
1	A	276	GLY	4.3
1	D	285	GLU	4.2
1	B	274	ASP	4.1
1	D	45	ARG	4.1
1	D	274	ASP	4.1
1	C	282	GLN	4.1
1	C	276	GLY	4.1
1	B	285	GLU	4.0
1	A	140	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	139	ASP	3.8
1	C	139	ASP	3.8
1	D	470	ASP	3.8
1	B	139	ASP	3.7
1	A	136	LYS	3.7
1	C	274	ASP	3.5
1	D	284	SER	3.5
1	D	140	GLN	3.4
1	C	469	ASP	3.4
1	A	137	ASP	3.3
1	B	249	ASN	3.3
1	A	271	MET	3.2
1	A	281	ASP	3.2
1	A	274	ASP	3.2
1	D	137	ASP	3.2
1	D	163	GLN	3.1
1	B	252	GLU	3.0
1	D	306	THR	3.0
1	C	306	THR	3.0
1	C	280	PRO	2.9
1	C	137	ASP	2.9
1	B	248	GLU	2.9
1	C	442	CYS	2.8
1	D	42	PHE	2.8
1	A	273	SER	2.8
1	C	470	ASP	2.8
1	A	138	GLY	2.7
1	B	140	GLN	2.7
1	A	257	ASP	2.7
1	C	47	GLY	2.7
1	C	310	VAL	2.7
1	A	304	VAL	2.6
1	A	306	THR	2.6
1	C	448	ALA	2.6
1	A	302	ALA	2.6
1	D	165	ILE	2.5
1	C	447	LEU	2.5
1	C	307	THR	2.5
1	A	206	ILE	2.5
1	D	340	ARG	2.5
1	D	407	HIS	2.5
1	B	253	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	307	THR	2.5
1	D	334	GLN	2.5
1	D	283	ASP	2.4
1	A	253	LYS	2.4
1	D	471	GLY	2.4
1	A	504	ALA	2.4
1	A	309	SER	2.4
1	C	43	LEU	2.4
1	A	483	VAL	2.3
1	D	310	VAL	2.3
1	A	497	GLN	2.3
1	D	472	GLN	2.3
1	A	308	THR	2.3
1	B	137	ASP	2.3
1	C	497	GLN	2.3
1	D	273	SER	2.3
1	C	493	ILE	2.3
1	B	134	LEU	2.3
1	C	501	GLU	2.3
1	B	175	VAL	2.2
1	A	452	LEU	2.2
1	D	339	SER	2.2
1	D	272	ASN	2.2
1	A	284	SER	2.2
1	D	448	ALA	2.2
1	C	500	ARG	2.2
1	A	119	ALA	2.2
1	D	420	PRO	2.2
1	C	367	ALA	2.1
1	C	41	PRO	2.1
1	D	500	ARG	2.1
1	D	419	ASN	2.1
1	A	285	GLU	2.1
1	B	304	VAL	2.1
1	C	248	GLU	2.1
1	D	308	THR	2.1
1	D	309	SER	2.1
1	B	301	GLY	2.1
1	A	310	VAL	2.0
1	C	283	ASP	2.0
1	C	308	THR	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](#)

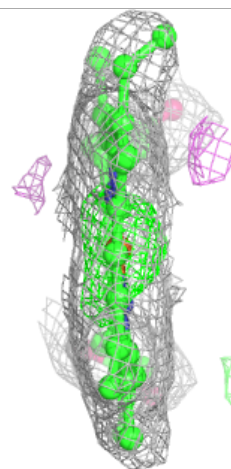
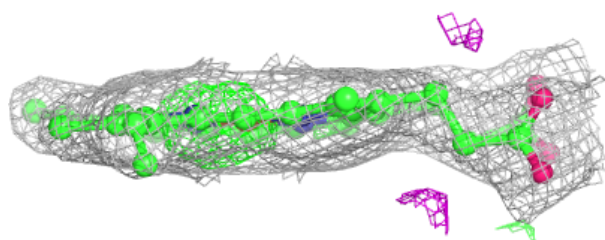
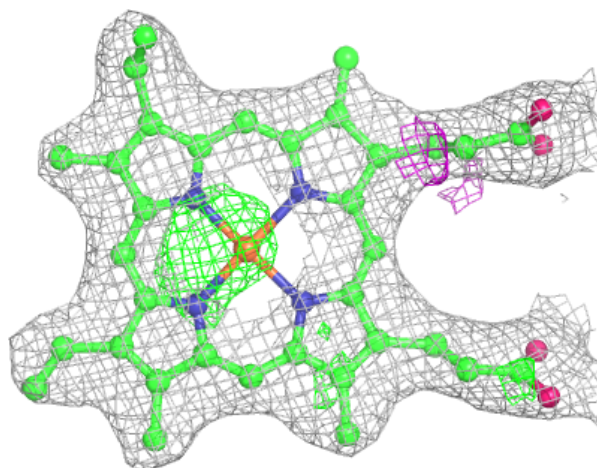
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	600	43/43	0.96	0.25	28,36,43,47	0
3	TOK	B	601	29/29	0.96	0.22	29,35,37,40	0
3	TOK	C	601	29/29	0.96	0.27	26,31,34,35	0
3	TOK	D	601	29/29	0.96	0.24	27,32,39,43	0
3	TOK	A	601	29/29	0.97	0.31	36,41,43,44	0
2	HEM	C	600	43/43	0.98	0.30	28,34,39,41	0
2	HEM	D	600	43/43	0.98	0.21	26,30,34,36	0
2	HEM	B	600	43/43	0.98	0.21	25,33,36,40	0

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

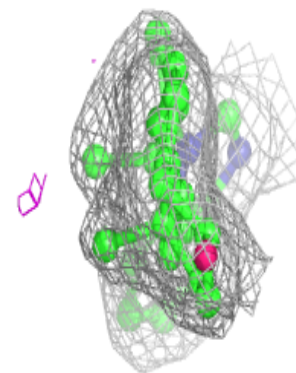
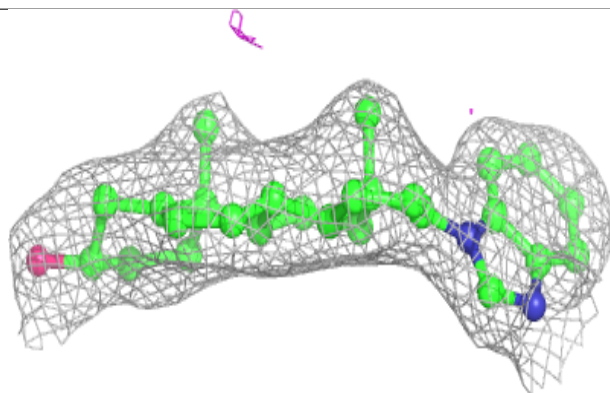
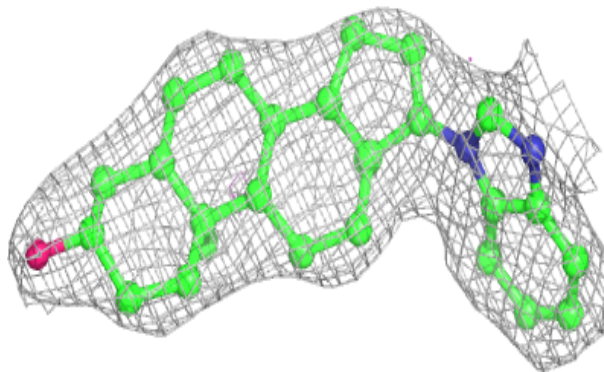
Electron density around HEM A 600:

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

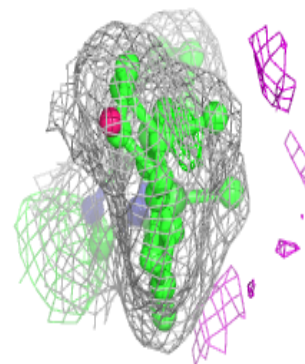
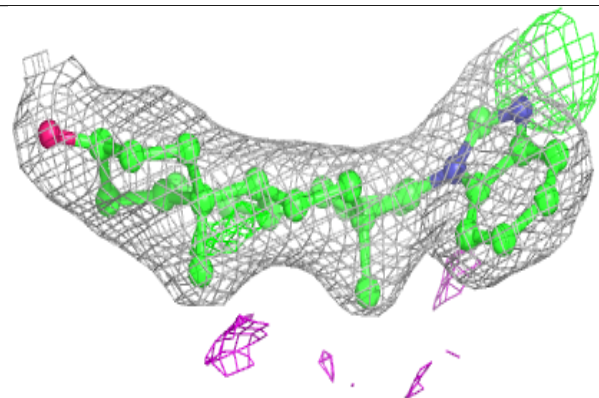
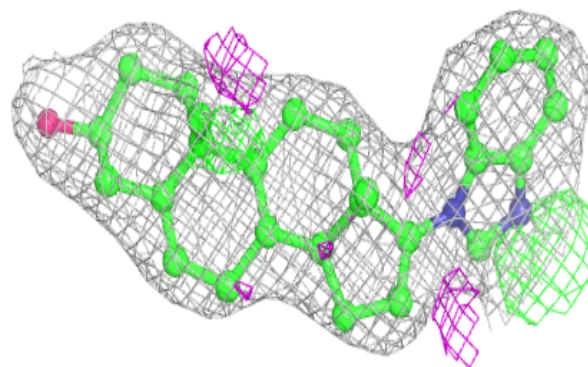


Electron density around TOK B 601:

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

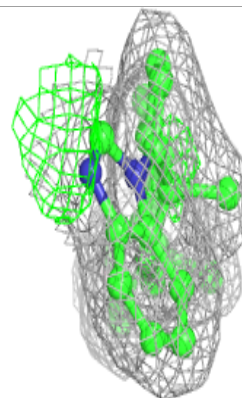
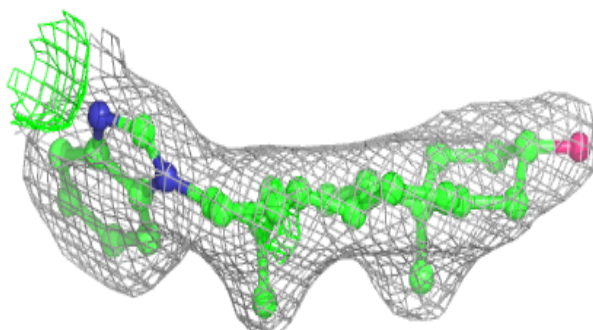
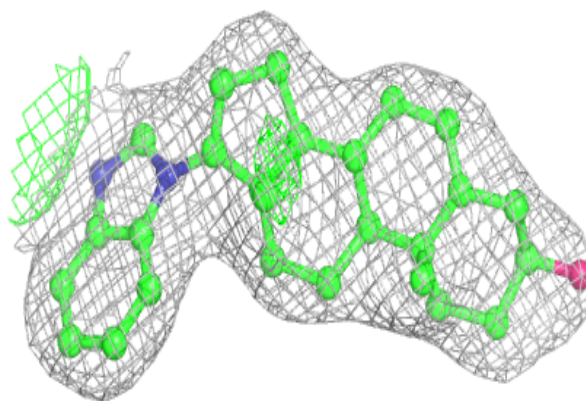
**Electron density around TOK C 601:**

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

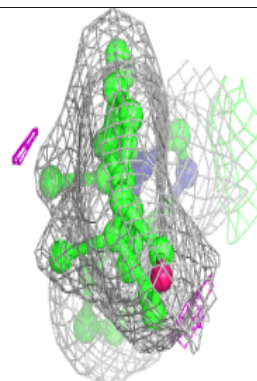
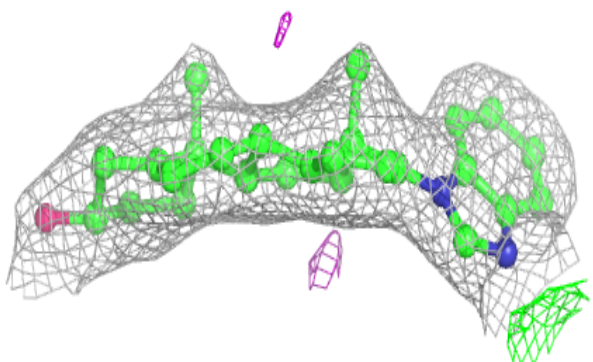
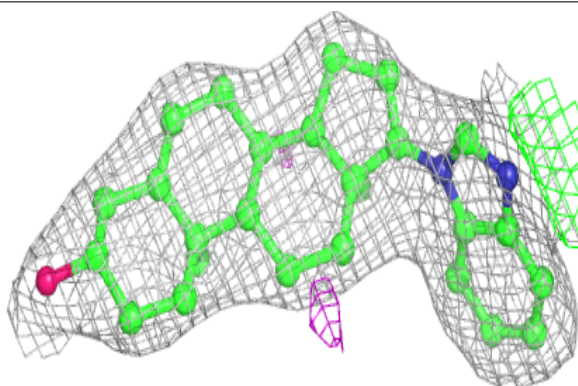


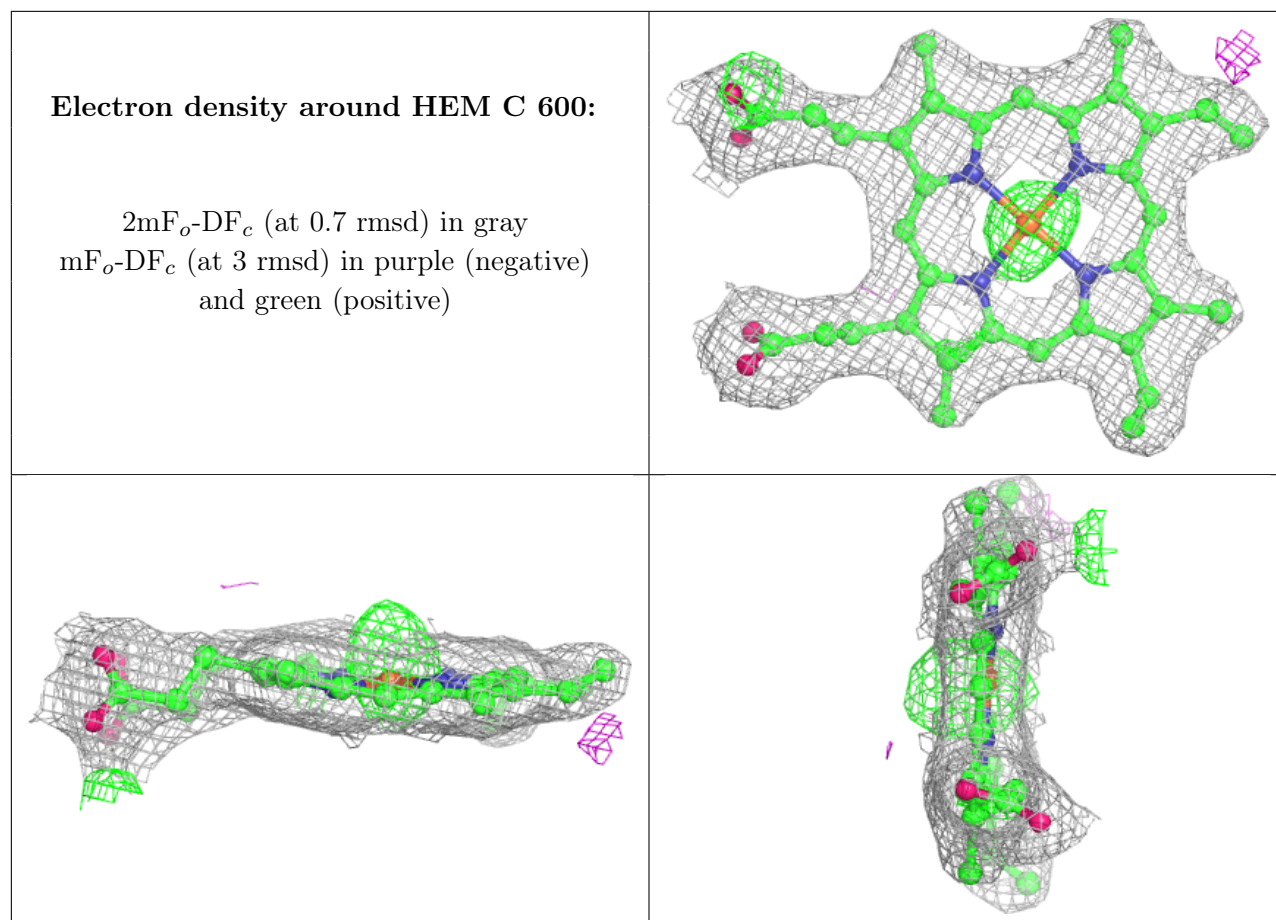
Electron density around TOK D 601:

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

**Electron density around TOK A 601:**

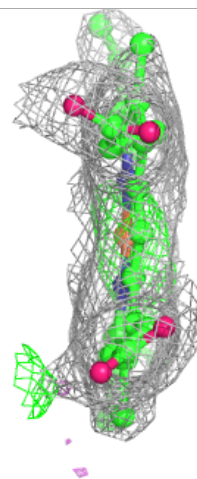
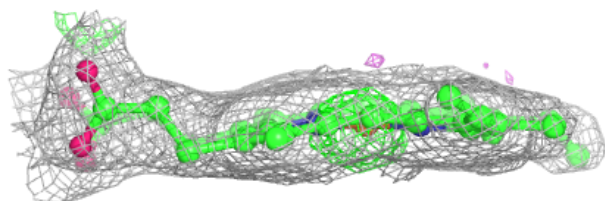
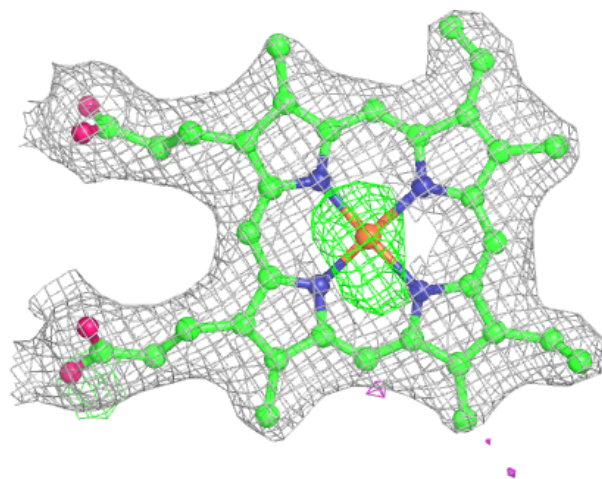
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

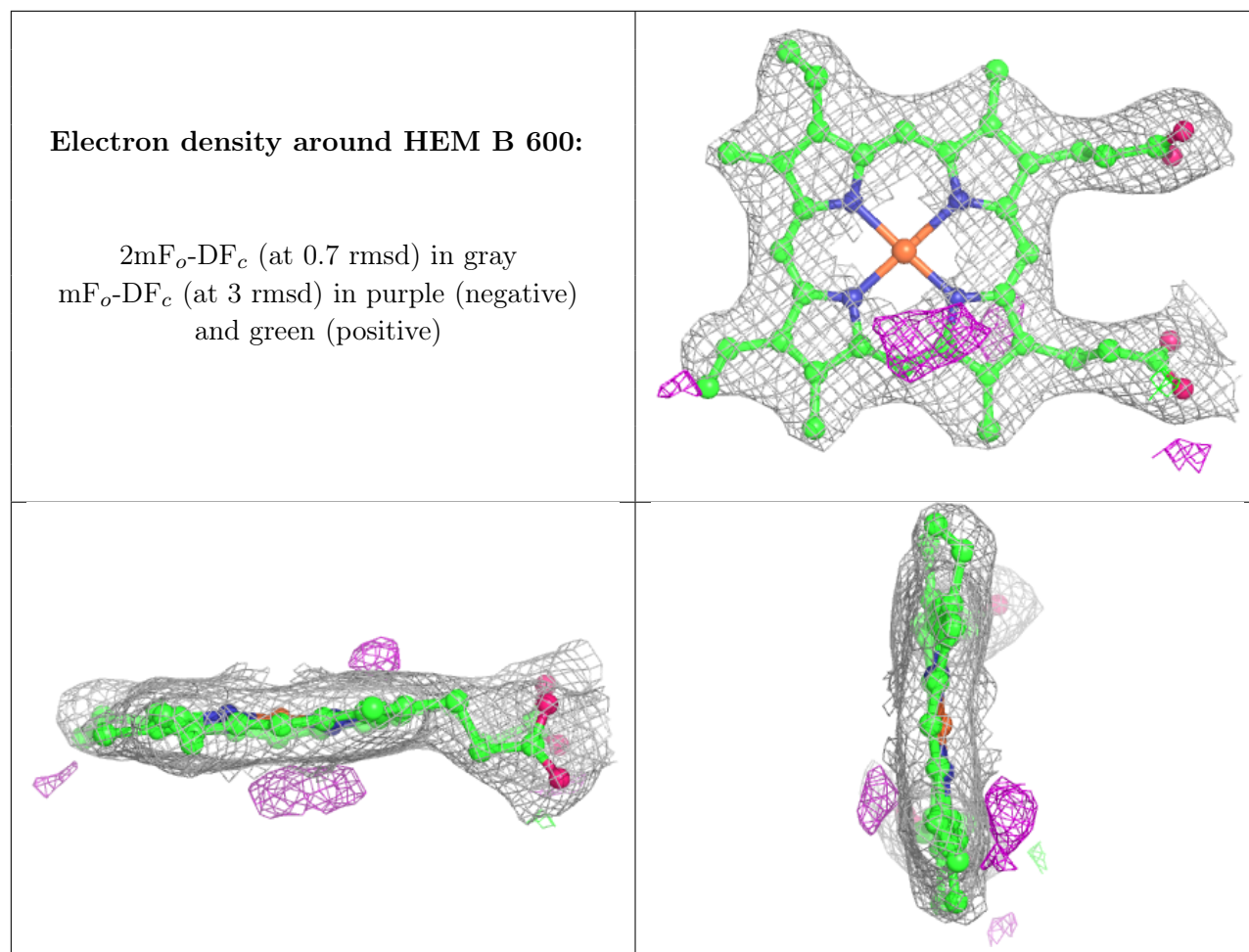




Electron density around HEM D 600:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.