



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:00 PM UTC

PDB ID : 3SWZ / pdb_00003swz
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	:	4-5-2 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

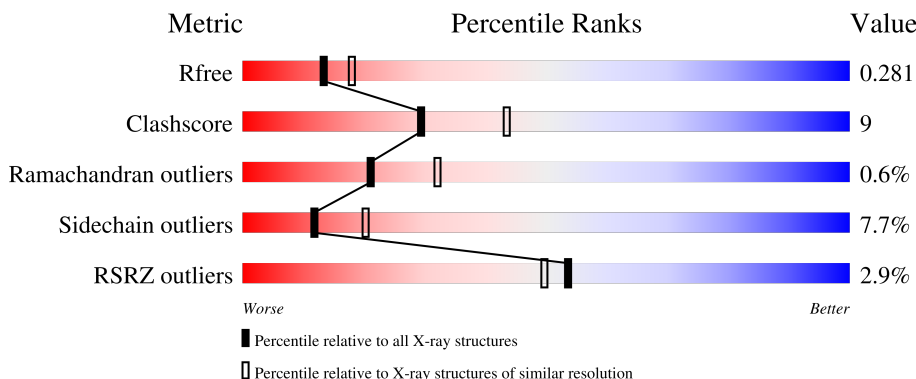
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	2% 76% 17% • 5%
1	B	494	2% 76% 16% • 6%
1	C	494	4% 71% 20% • 5%
1	D	494	4% 68% 22% • 6%

2 Entry composition

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

There are 36 discrepancies between the modelled and reference sequences:

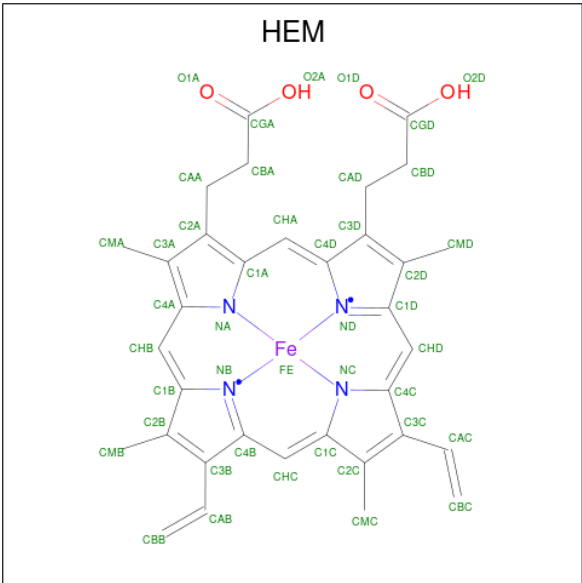
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP 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 (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



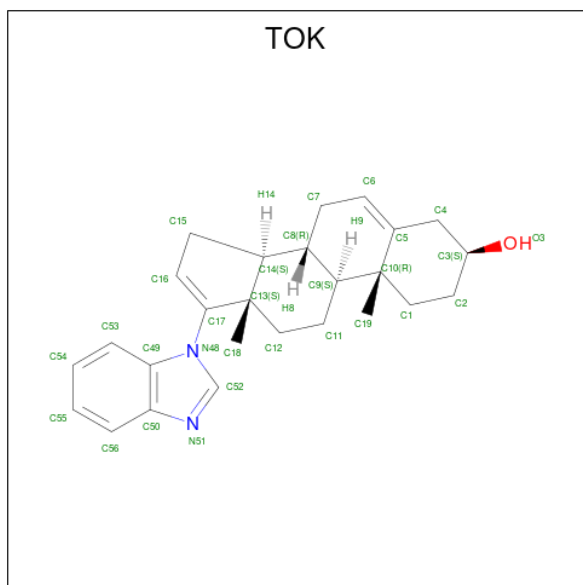
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

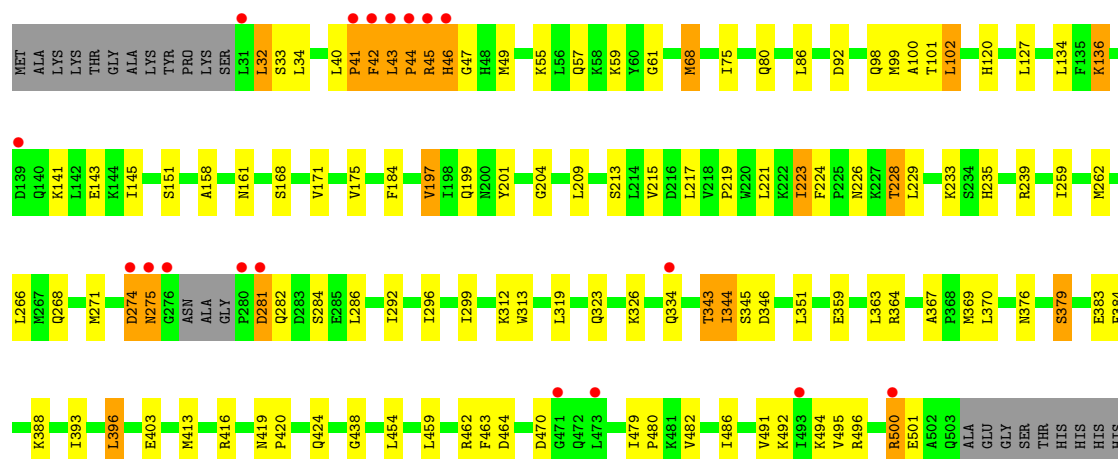
- Molecule 3 is (3alpha,8alpha)-17-(1H-benzimidazol-1-yl)androsta-5,16-dien-3-ol (CCD ID: TOK) (formula: C₂₆H₃₂N₂O).



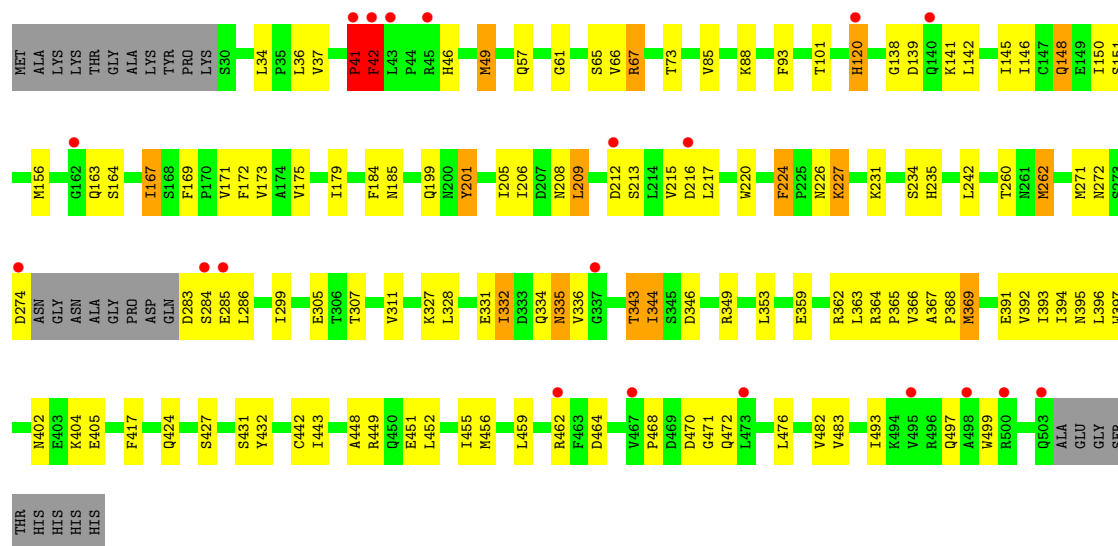
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	26	2	1		
3	B	1	Total	C	N	O	0	0
			29	26	2	1		
3	C	1	Total	C	N	O	0	0
			29	26	2	1		
3	D	1	Total	C	N	O	0	0
			29	26	2	1		

- 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		



• 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) 99.9 (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)	Xtriage
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	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15296	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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	0.97	3/3828 (0.1%)	1.12	12/5182 (0.2%)
1	B	0.97	2/3788 (0.1%)	1.13	7/5128 (0.1%)
1	C	1.02	0/3834	1.18	13/5190 (0.3%)
1	D	0.95	0/3794	1.17	13/5136 (0.3%)
All	All	0.98	5/15244 (0.0%)	1.15	45/20636 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASP	C-O	13.73	1.33	1.23
1	A	72	THR	CA-CB	7.01	1.64	1.53
1	B	212	ASP	C-O	6.61	1.32	1.24
1	A	314	THR	CA-CB	5.26	1.61	1.53
1	B	491	VAL	CA-CB	5.04	1.61	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	PRO	CA-N-CD	-9.42	98.81	112.00
1	C	47	GLY	N-CA-C	8.80	121.76	111.63
1	B	137	ASP	N-CA-C	8.48	121.27	108.46
1	D	427	SER	CA-C-N	8.39	128.04	119.82
1	D	427	SER	C-N-CA	8.39	128.04	119.82
1	C	223	ILE	N-CA-C	7.67	118.46	110.72
1	D	46	HIS	N-CA-C	7.53	121.81	112.47
1	C	463	PHE	N-CA-C	6.80	120.25	108.76
1	A	118	GLY	N-CA-C	6.64	119.40	110.43
1	A	262	MET	N-CA-C	6.53	118.40	111.28
1	A	192	ASP	CA-C-N	6.44	126.37	119.28
1	A	192	ASP	C-N-CA	6.44	126.37	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	ILE	N-CA-C	-6.22	105.66	111.45
1	D	220	TRP	N-CA-C	6.16	118.78	111.33
1	A	438	GLY	CA-C-N	6.08	125.76	119.56
1	A	438	GLY	C-N-CA	6.08	125.76	119.56
1	B	482	VAL	CB-CA-C	-6.02	102.84	112.16
1	C	197	VAL	N-CA-C	-5.91	104.75	110.42
1	D	42	PHE	N-CA-C	5.91	118.79	109.39
1	C	43	LEU	CA-C-N	-5.84	112.54	119.84
1	C	43	LEU	C-N-CA	-5.84	112.54	119.84
1	B	470	ASP	N-CA-C	-5.77	101.31	109.96
1	D	262	MET	N-CA-C	5.76	117.56	111.28
1	A	491	VAL	CB-CA-C	-5.62	101.84	110.50
1	A	408	GLN	CA-C-N	5.54	125.37	119.28
1	A	408	GLN	C-N-CA	5.54	125.37	119.28
1	C	496	ARG	N-CA-C	5.50	117.83	110.35
1	D	224	PHE	CA-C-N	5.47	126.67	119.84
1	D	224	PHE	C-N-CA	5.47	126.67	119.84
1	A	113	ALA	N-CA-C	5.43	117.20	111.28
1	C	274	ASP	N-CA-C	-5.35	102.74	111.04
1	D	209	LEU	N-CA-C	5.30	117.14	111.36
1	D	139	ASP	N-CA-C	-5.29	105.41	111.07
1	D	34	LEU	CA-C-N	-5.22	114.42	119.90
1	D	34	LEU	C-N-CA	-5.22	114.42	119.90
1	A	152	THR	N-CA-C	5.15	116.58	111.07
1	B	321	ASN	CA-C-N	5.13	124.93	119.28
1	B	321	ASN	C-N-CA	5.13	124.93	119.28
1	C	49	MET	N-CA-C	5.13	117.61	111.71
1	C	281	ASP	N-CA-C	5.07	116.80	111.28
1	B	491	VAL	CB-CA-C	-5.03	102.99	110.33
1	B	220	TRP	N-CA-C	5.03	117.41	111.33
1	A	394	ILE	CB-CA-C	-5.02	104.89	110.96
1	C	41	PRO	CA-C-N	5.01	128.58	121.42
1	C	41	PRO	C-N-CA	5.01	128.58	121.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3810	52	0
1	B	3708	0	3779	50	0
1	C	3750	0	3816	74	0
1	D	3714	0	3784	88	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	2	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	264	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 9.

All (264) 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:B:68:MET:HE1	1:C:40:LEU:HD12	1.39	1.01
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:A:40:LEU:HD21	1:A:68:MET:HE1	1.68	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:213:SER:HB2	1:D:369:MET:HE3	1.75	0.67
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:D:49:MET:HB2	1:D:212:ASP:CG	2.22	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:B:211:LYS:HD3	1:B:211:LYS:C	2.26	0.60
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: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
1:D:284:SER:C	1:D:286:LEU:H	2.12	0.58
2:D:600:HEM:C1B	3:D:601:TOK:H56	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:273:SER:OG	1:B:274:ASP:N	2.30	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:D:65:SER:HA	1:D:73:THR:O	2.08	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:C:213:SER:HB2	1:C:369:MET:HE3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:99:MET:O	1:C:100:ALA:C	2.53	0.51
1:A:500:ARG:HG3	1:A:500:ARG:HH11	1.74	0.51
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:B:68:MET:HE1	1:C:40:LEU:CD1	2.25	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:D:242:LEU:HD23	1:D:242:LEU:C	2.37	0.49
1:A:501:GLU:C	1:A:503:GLN:H	2.19	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:A:211:LYS:HD3	1:A:211:LYS:C	2.37	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: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:A:221:LEU:HD12	1:A:221:LEU:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:34:LEU:HD12	1:C:34:LEU:C	2.40	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
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: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: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: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:212:ASP:CG	1:D:213:SER:H	2.25	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:43:LEU:C	1:C:44:PRO:O	2.60	0.45
1:C:86:LEU:O	1:C:438:GLY:HA3	2.17	0.45
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:A:106:SER:O	1:A:107:ASN:C	2.60	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:A:271:MET:C	1:A:273:SER:H	2.27	0.43
1:D:120:HIS:CD2	1:D:120:HIS:H	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:212:ASP:CG	1:D:213:SER:N	2.77	0.43
1:A:174:ALA:O	1:A:178:VAL:HG23	2.19	0.43
1:D:201:TYR:CD1	1:D:201:TYR:C	2.97	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:261:ASN:OD1	1:A:261:ASN:C	2.61	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:C:274:ASP:O	1:C:275:ASN:C	2.61	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: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:C:43:LEU:O	1:C:44:PRO:C	2.61	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:A:460:LEU:O	1:A:461:GLN:C	2.61	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:A:494:LYS:NZ	4:A:520:HOH:O	2.52	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:172:PHE:CD2	1:B:172:PHE:C	2.98	0.42
1:B:214:LEU:HD11	1:B:482:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:172:PHE:CD2	1:D:172:PHE:C	2.98	0.41
1:A:101:THR:HG23	1:A:102:LEU:N	2.35	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
1:C:68:MET:HE3	1:C:217:LEU:HD22	2.03	0.41
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:74:VAL:C	1:A:75:ILE:HD12	2.46	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:C:282:GLN:CD	1:C:282:GLN:H	2.29	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:B:470:ASP:O	1:B:470:ASP:CG	2.63	0.40
1:D:208:ASN:OD1	1:D:231:LYS:HE3	2.20	0.40
1:B:261:ASN:C	1:B:261:ASN:OD1	2.63	0.40
1:C:482:VAL:O	3:C:601:TOK:H54	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	58
1	B	461/494 (93%)	434 (94%)	27 (6%)	0	100	100
1	C	467/494 (94%)	433 (93%)	28 (6%)	6 (1%)	9	14
1	D	462/494 (94%)	414 (90%)	43 (9%)	5 (1%)	11	18
All	All	1857/1976 (94%)	1724 (93%)	121 (6%)	12 (1%)	21	32

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 ⓘ

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%)	16	28
1	B	415/436 (95%)	384 (92%)	31 (8%)	12	21
1	C	420/436 (96%)	381 (91%)	39 (9%)	8	14
1	D	416/436 (95%)	384 (92%)	32 (8%)	12	20
All	All	1670/1744 (96%)	1541 (92%)	129 (8%)	12	20

All (129) 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	179	ILE
1	A	180	SER
1	A	211	LYS
1	A	221	LEU
1	A	227	LYS
1	A	234	SER
1	A	255	ARG
1	A	271	MET
1	A	281	ASP
1	A	285	GLU
1	A	307	THR
1	A	319	LEU
1	A	334	GLN
1	A	343	THR
1	A	344	ILE
1	A	363	LEU
1	A	396	LEU
1	A	399	LEU
1	A	408	GLN

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Mol	Chain	Res	Type
1	A	459	LEU
1	A	482	VAL
1	A	491	VAL
1	B	37	VAL
1	B	70	THR
1	B	71	LYS
1	B	72	THR
1	B	80	GLN
1	B	91	LYS
1	B	98	GLN
1	B	120	HIS
1	B	172	PHE
1	B	182	ILE
1	B	207	ASP
1	B	211	LYS
1	B	217	LEU
1	B	236	VAL
1	B	253	LYS
1	B	255	ARG
1	B	274	ASP
1	B	307	THR
1	B	319	LEU
1	B	330	GLU
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	459	LEU
1	B	482	VAL
1	B	501	GLU
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

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Mol	Chain	Res	Type
1	C	102	LEU
1	C	136	LYS
1	C	143	GLU
1	C	145	ILE
1	C	151	SER
1	C	197	VAL
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	351	LEU
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	462	ARG
1	C	464	ASP
1	C	470	ASP
1	C	491	VAL
1	C	500	ARG
1	C	501	GLU
1	D	37	VAL
1	D	42	PHE
1	D	49	MET
1	D	67	ARG
1	D	88	LYS
1	D	120	HIS
1	D	145	ILE
1	D	148	GLN
1	D	151	SER
1	D	156	MET
1	D	163	GLN

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Mol	Chain	Res	Type
1	D	167	ILE
1	D	179	ILE
1	D	199	GLN
1	D	201	TYR
1	D	227	LYS
1	D	234	SER
1	D	271	MET
1	D	327	LYS
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	369	MET
1	D	396	LEU
1	D	431	SER
1	D	449	ARG
1	D	459	LEU
1	D	464	ASP
1	D	482	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	79	HIS
1	A	200	ASN
1	A	275	ASN
1	A	335	ASN
1	B	78	HIS
1	B	140	GLN
1	B	190	ASN
1	B	199	GLN
1	B	402	ASN
1	C	50	HIS
1	C	57	GLN
1	C	79	HIS
1	C	148	GLN
1	C	235	HIS
1	C	268	GLN
1	C	275	ASN

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Mol	Chain	Res	Type
1	C	450	GLN
1	C	472	GLN
1	C	503	GLN
1	D	57	GLN
1	D	148	GLN
1	D	199	GLN
1	D	320	HIS
1	D	335	ASN
1	D	401	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	TOK	D	601	2	33,34,34	1.27	4 (12%)	48,54,54	3.71	12 (25%)
3	TOK	C	601	2	33,34,34	1.39	3 (9%)	48,54,54	3.91	18 (37%)
2	HEM	A	600	3,1	50,50,50	1.93	10 (20%)	67,82,82	1.47	11 (16%)
3	TOK	B	601	2	33,34,34	1.26	4 (12%)	48,54,54	4.07	16 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	600	3,1	50,50,50	1.77	8 (16%)	67,82,82	1.57	12 (17%)
3	TOK	A	601	2	33,34,34	1.17	3 (9%)	48,54,54	3.42	15 (31%)
2	HEM	C	600	3,1	50,50,50	2.03	14 (28%)	67,82,82	1.56	11 (16%)
2	HEM	D	600	3,1	50,50,50	1.88	11 (22%)	67,82,82	1.28	8 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TOK	D	601	2	-	1/2/62/62	0/6/6/6
3	TOK	C	601	2	-	0/2/62/62	0/6/6/6
2	HEM	A	600	3,1	-	2/14/54/54	-
3	TOK	B	601	2	-	0/2/62/62	0/6/6/6
2	HEM	B	600	3,1	-	5/14/54/54	-
3	TOK	A	601	2	-	1/2/62/62	0/6/6/6
2	HEM	C	600	3,1	-	3/14/54/54	-
2	HEM	D	600	3,1	-	7/14/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3D-C2D	7.78	1.53	1.36
2	C	600	HEM	C3D-C2D	7.73	1.53	1.36
2	D	600	HEM	C3D-C2D	7.18	1.52	1.36
2	B	600	HEM	C3D-C2D	6.56	1.50	1.36
3	C	601	TOK	C49-N48	-5.69	1.32	1.40
2	A	600	HEM	FE-ND	5.49	2.11	1.94
2	C	600	HEM	FE-NB	5.19	2.10	1.94
2	C	600	HEM	FE-ND	5.16	2.10	1.94
2	B	600	HEM	FE-ND	4.84	2.09	1.94
2	C	600	HEM	FE-NC	4.51	2.10	1.95
3	B	601	TOK	C52-N48	-3.82	1.31	1.37
3	D	601	TOK	C52-N48	-3.69	1.32	1.37
2	D	600	HEM	CAB-C3B	3.53	1.56	1.47
2	A	600	HEM	CAC-C3C	3.51	1.56	1.47
2	A	600	HEM	CAB-C3B	3.34	1.56	1.47
2	D	600	HEM	FE-NB	3.30	2.05	1.94
2	A	600	HEM	FE-NA	3.28	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	C1B-NB	-3.17	1.34	1.40
3	B	601	TOK	C49-N48	-3.11	1.36	1.40
3	D	601	TOK	C49-N48	-3.09	1.36	1.40
3	A	601	TOK	C52-N48	-2.98	1.33	1.37
3	A	601	TOK	C49-N48	-2.97	1.36	1.40
2	D	600	HEM	CMD-C2D	2.96	1.56	1.50
2	D	600	HEM	FE-ND	2.95	2.04	1.94
2	C	600	HEM	FE-NA	2.89	2.04	1.95
2	D	600	HEM	CAC-C3C	2.83	1.54	1.47
2	B	600	HEM	CAB-C3B	2.79	1.54	1.47
2	C	600	HEM	CAC-C3C	2.74	1.54	1.47
2	A	600	HEM	C1A-NA	-2.52	1.34	1.39
3	D	601	TOK	C52-N51	2.51	1.36	1.31
2	C	600	HEM	CAB-C3B	2.50	1.54	1.47
3	D	601	TOK	C50-N51	-2.49	1.35	1.39
2	B	600	HEM	CAC-C3C	2.45	1.53	1.47
3	A	601	TOK	C50-N51	-2.44	1.35	1.39
3	C	601	TOK	C50-N51	-2.43	1.35	1.39
2	C	600	HEM	CAA-C2A	2.37	1.57	1.51
2	C	600	HEM	CMB-C2B	2.36	1.55	1.50
2	D	600	HEM	CMA-C3A	2.32	1.55	1.50
2	C	600	HEM	CMA-C3A	2.31	1.55	1.50
3	B	601	TOK	C54-C53	2.31	1.42	1.38
2	A	600	HEM	CHC-C4B	-2.28	1.34	1.39
2	B	600	HEM	CMB-C2B	2.27	1.55	1.50
2	C	600	HEM	CMC-C2C	2.26	1.55	1.50
2	A	600	HEM	CAA-C2A	2.26	1.57	1.51
2	D	600	HEM	CMB-C2B	2.23	1.55	1.50
2	B	600	HEM	CHB-C1B	-2.19	1.34	1.38
2	C	600	HEM	CMD-C2D	2.14	1.55	1.50
2	B	600	HEM	CMA-C3A	2.14	1.55	1.50
3	B	601	TOK	C15-C16	2.12	1.53	1.50
2	C	600	HEM	C3C-C2C	-2.10	1.32	1.37
3	C	601	TOK	C52-N48	-2.09	1.34	1.37
2	D	600	HEM	O2D-CGD	-2.09	1.23	1.30
2	A	600	HEM	FE-NB	2.09	2.01	1.94
2	D	600	HEM	C4D-ND	-2.08	1.36	1.40
2	B	600	HEM	CMC-C2C	2.06	1.55	1.50
2	A	600	HEM	C1B-NB	-2.02	1.36	1.40
2	C	600	HEM	O2A-CGA	-2.01	1.24	1.30

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	TOK	C49-N48-C52	20.50	113.68	105.95
3	C	601	TOK	C49-N48-C52	19.57	113.33	105.95
3	D	601	TOK	C49-N48-C52	18.40	112.89	105.95
3	A	601	TOK	C49-N48-C52	15.70	111.87	105.95
3	B	601	TOK	N48-C52-N51	-14.40	105.69	113.88
3	D	601	TOK	N48-C52-N51	-14.31	105.74	113.88
3	C	601	TOK	N48-C52-N51	-12.76	106.62	113.88
3	A	601	TOK	N48-C52-N51	-12.62	106.70	113.88
3	C	601	TOK	C3-C4-C5	-6.05	102.42	112.05
2	C	600	HEM	C4D-ND-C1D	6.04	112.36	105.21
2	B	600	HEM	C4D-ND-C1D	5.54	111.77	105.21
2	A	600	HEM	C4D-ND-C1D	5.40	111.60	105.21
3	B	601	TOK	C50-N51-C52	4.92	110.43	104.40
3	D	601	TOK	C50-N51-C52	4.69	110.15	104.40
3	C	601	TOK	C7-C8-C9	4.64	115.08	109.72
3	A	601	TOK	C15-C14-C13	4.15	106.95	104.05
3	B	601	TOK	C53-C49-N48	4.12	137.91	130.46
3	A	601	TOK	C50-N51-C52	4.07	109.40	104.40
2	D	600	HEM	C4D-ND-C1D	3.96	109.90	105.21
3	B	601	TOK	C15-C14-C13	-3.93	101.29	104.05
2	B	600	HEM	CHD-C4C-NC	3.92	128.72	124.45
3	B	601	TOK	C1-C2-C3	3.74	115.43	110.48
2	D	600	HEM	C3B-C2B-C1B	3.71	109.19	106.41
3	C	601	TOK	C7-C8-C14	3.57	115.99	110.93
3	A	601	TOK	C14-C8-C9	-3.57	104.42	109.09
3	A	601	TOK	C53-C49-N48	3.43	136.67	130.46
2	B	600	HEM	CAA-CBA-CGA	-3.42	104.59	113.67
3	B	601	TOK	C3-C4-C5	-3.36	106.69	112.05
3	C	601	TOK	C50-N51-C52	3.33	108.49	104.40
3	D	601	TOK	C53-C49-N48	3.31	136.45	130.46
3	C	601	TOK	C50-C49-N48	-3.19	102.63	104.95
3	A	601	TOK	C3-C4-C5	-3.18	106.98	112.05
2	D	600	HEM	CHC-C1C-NC	3.17	127.90	124.45
3	C	601	TOK	C19-C10-C1	3.17	114.25	109.43
2	A	600	HEM	O2A-CGA-CBA	3.07	123.70	114.00
2	D	600	HEM	C1D-C2D-C3D	-3.04	103.78	106.98
3	D	601	TOK	C4-C5-C6	-3.04	116.45	120.57
2	C	600	HEM	C2A-C1A-NA	-3.02	106.80	110.15
3	B	601	TOK	C53-C49-C50	-3.01	118.75	122.23
3	A	601	TOK	C12-C11-C9	3.01	118.25	113.14
2	B	600	HEM	C4C-C3C-C2C	2.99	109.40	106.81
2	C	600	HEM	C3B-C2B-C1B	2.97	108.64	106.41
3	D	601	TOK	C15-C14-C13	2.95	106.11	104.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	TOK	C1-C2-C3	-2.94	106.59	110.48
3	C	601	TOK	C53-C49-N48	2.92	135.74	130.46
3	B	601	TOK	C49-C50-N51	-2.91	106.86	110.00
2	B	600	HEM	CAD-C3D-C4D	2.90	129.75	124.70
3	D	601	TOK	C49-C50-N51	-2.77	107.00	110.00
2	A	600	HEM	O1A-CGA-CBA	-2.74	114.40	123.09
3	C	601	TOK	C4-C5-C10	2.74	119.93	116.42
3	A	601	TOK	C19-C10-C1	2.71	113.56	109.43
3	A	601	TOK	C53-C49-C50	-2.71	119.11	122.23
2	A	600	HEM	CMA-C3A-C4A	-2.67	121.35	125.42
2	D	600	HEM	O2A-CGA-CBA	2.66	122.39	114.00
3	D	601	TOK	C18-C13-C12	-2.62	108.11	111.10
3	C	601	TOK	C12-C13-C14	-2.62	104.82	108.88
2	C	600	HEM	C1B-NB-C4B	2.59	108.28	105.21
2	D	600	HEM	CMD-C2D-C1D	2.58	129.06	125.03
2	C	600	HEM	C3D-C4D-ND	-2.57	107.36	110.17
2	A	600	HEM	CMA-C3A-C2A	2.54	131.01	125.62
3	C	601	TOK	C19-C10-C9	-2.53	108.82	111.66
3	D	601	TOK	C53-C49-C50	-2.53	119.31	122.23
2	B	600	HEM	CHD-C1D-ND	2.50	127.11	124.42
3	B	601	TOK	C2-C1-C10	2.48	118.07	112.78
2	A	600	HEM	C3C-C2C-C1C	2.47	109.38	107.05
2	A	600	HEM	CAD-C3D-C4D	2.47	129.00	124.70
2	C	600	HEM	C3B-C4B-NB	-2.46	107.70	109.47
3	C	601	TOK	C4-C5-C6	-2.44	117.26	120.57
3	D	601	TOK	C3-C4-C5	-2.44	108.17	112.05
2	C	600	HEM	C4A-NA-C1A	2.43	109.79	105.82
3	A	601	TOK	C7-C8-C14	2.43	114.38	110.93
3	B	601	TOK	C18-C13-C14	-2.43	109.51	112.99
3	C	601	TOK	C9-C10-C5	2.36	113.11	109.65
3	C	601	TOK	C18-C13-C14	2.35	116.37	112.99
2	A	600	HEM	C4D-C3D-C2D	-2.31	103.54	106.89
2	B	600	HEM	O2A-CGA-CBA	2.30	121.28	114.00
3	D	601	TOK	C4-C5-C10	2.29	119.36	116.42
3	A	601	TOK	C1-C10-C9	-2.28	105.72	108.74
3	A	601	TOK	C11-C9-C8	2.26	114.94	111.78
3	B	601	TOK	C50-C49-N48	-2.23	103.33	104.95
2	A	600	HEM	CMB-C2B-C1B	-2.23	121.56	125.03
3	C	601	TOK	C19-C10-C5	-2.22	104.99	108.38
3	B	601	TOK	C7-C8-C14	2.21	114.06	110.93
2	B	600	HEM	CBC-CAC-C3C	-2.21	116.48	127.53
2	C	600	HEM	CHA-C4D-ND	2.19	127.07	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	TOK	C19-C10-C9	-2.18	109.22	111.66
2	B	600	HEM	CMD-C2D-C1D	2.15	128.40	125.03
2	A	600	HEM	CHC-C1C-NC	2.15	126.79	124.45
2	D	600	HEM	CBA-CAA-C2A	2.15	118.47	112.53
2	C	600	HEM	C2B-C1B-NB	-2.13	107.39	109.84
3	B	601	TOK	C15-C14-C8	-2.13	119.38	121.63
3	B	601	TOK	C19-C10-C1	2.12	112.65	109.43
2	B	600	HEM	CAD-C3D-C2D	-2.11	123.92	127.87
2	B	600	HEM	C3D-C4D-ND	-2.09	107.87	110.17
3	C	601	TOK	C14-C8-C9	-2.07	106.38	109.09
2	B	600	HEM	C2A-C1A-NA	-2.07	107.86	110.15
2	C	600	HEM	CHB-C4A-NA	2.05	127.59	123.86
2	A	600	HEM	CMD-C2D-C1D	2.05	128.24	125.03
2	C	600	HEM	CHC-C1C-NC	2.05	126.69	124.45
2	D	600	HEM	O1A-CGA-CBA	-2.05	116.59	123.09
3	A	601	TOK	C1-C2-C3	2.04	113.19	110.48
3	D	601	TOK	C14-C13-C17	-2.03	97.08	100.28
3	A	601	TOK	C49-C50-N51	-2.02	107.81	110.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

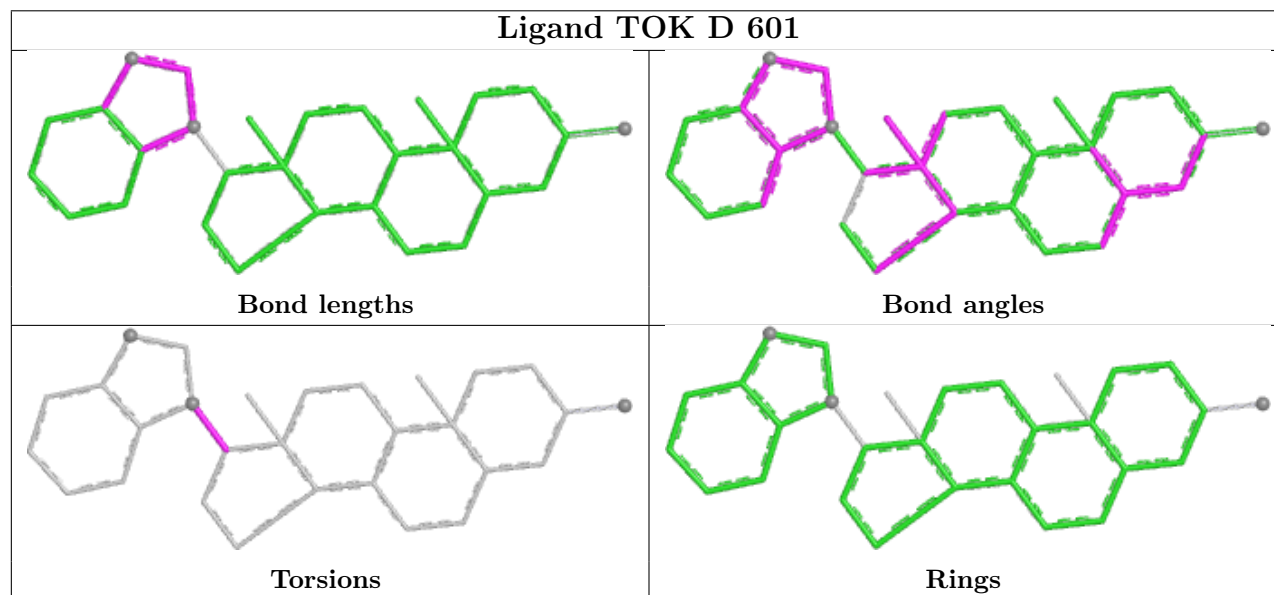
Mol	Chain	Res	Type	Atoms
2	A	600	HEM	C2C-C3C-CAC-CBC
2	D	600	HEM	C2B-C3B-CAB-CBB
2	C	600	HEM	C2C-C3C-CAC-CBC
2	A	600	HEM	C4C-C3C-CAC-CBC
2	D	600	HEM	C4B-C3B-CAB-CBB
2	B	600	HEM	C2C-C3C-CAC-CBC
3	A	601	TOK	C16-C17-N48-C52
3	D	601	TOK	C16-C17-N48-C52
2	C	600	HEM	C4C-C3C-CAC-CBC
2	B	600	HEM	CAA-CBA-CGA-O1A
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	D	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	C4C-C3C-CAC-CBC
2	B	600	HEM	CAD-CBD-CGD-O2D
2	C	600	HEM	CAD-CBD-CGD-O2D

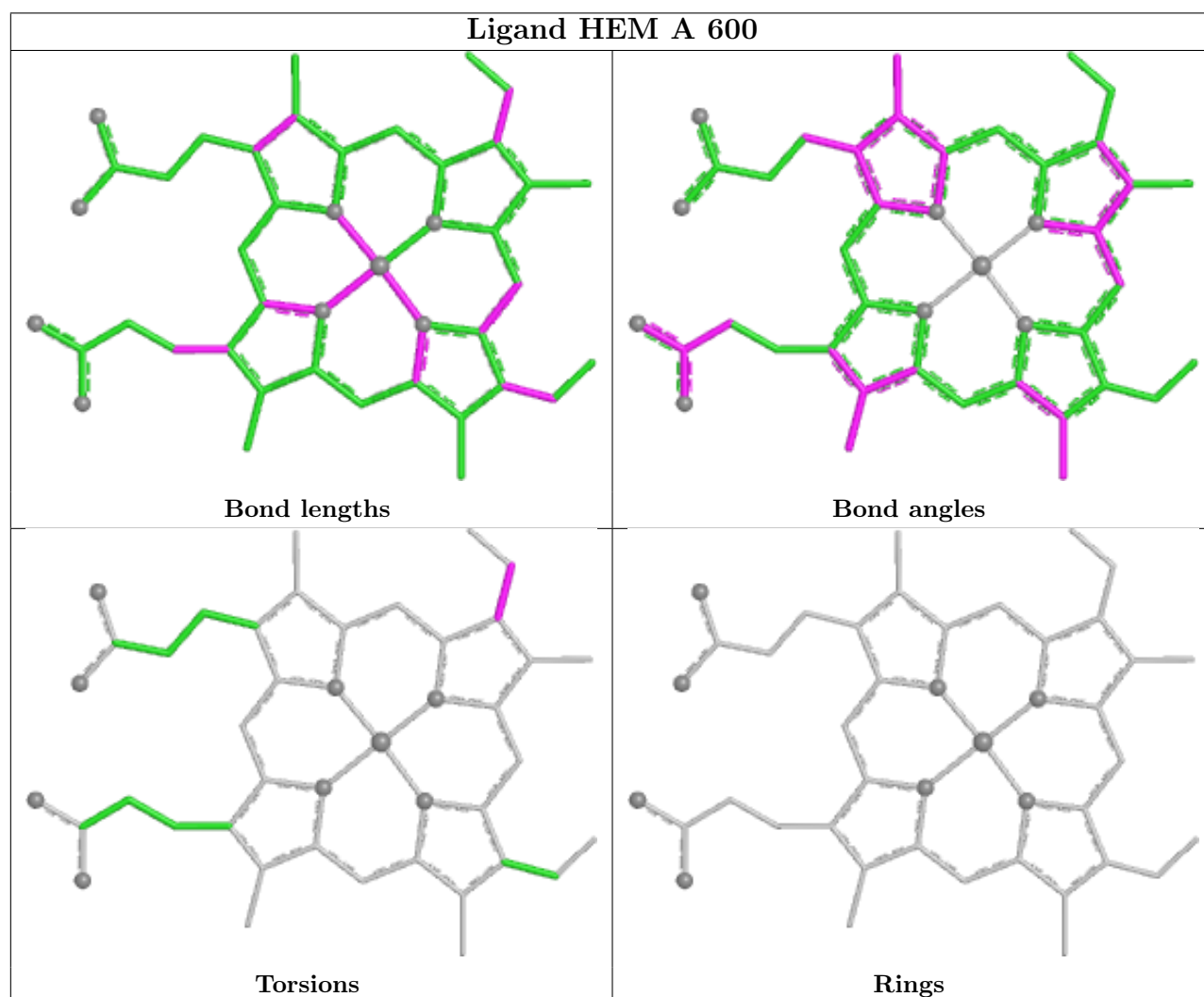
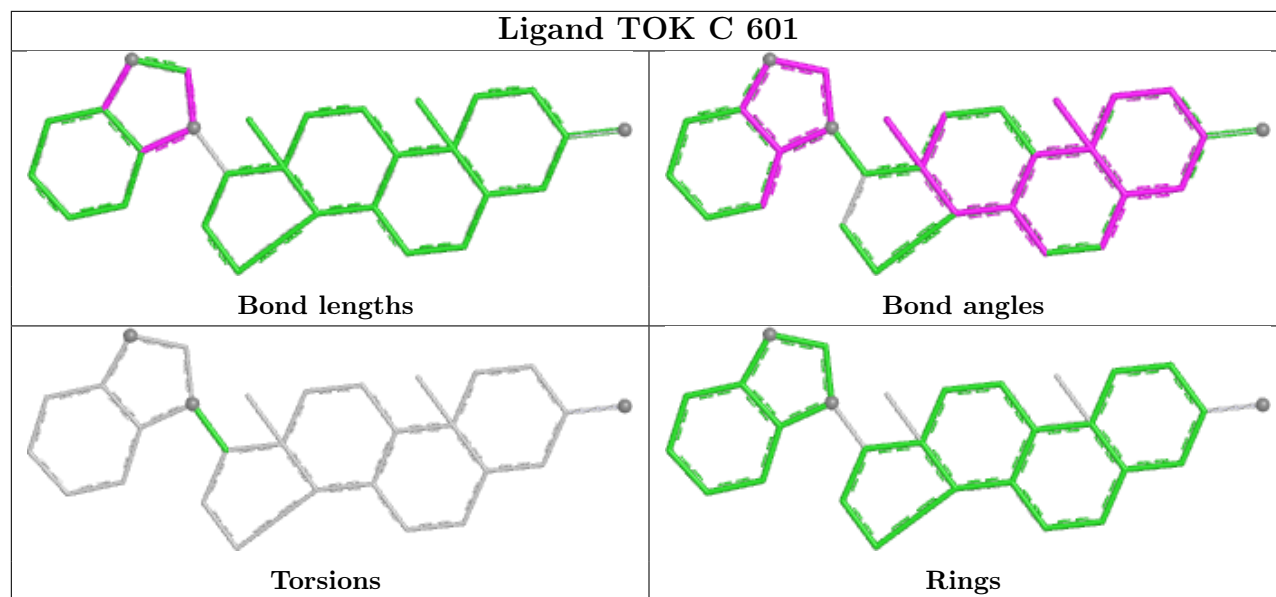
There are no ring outliers.

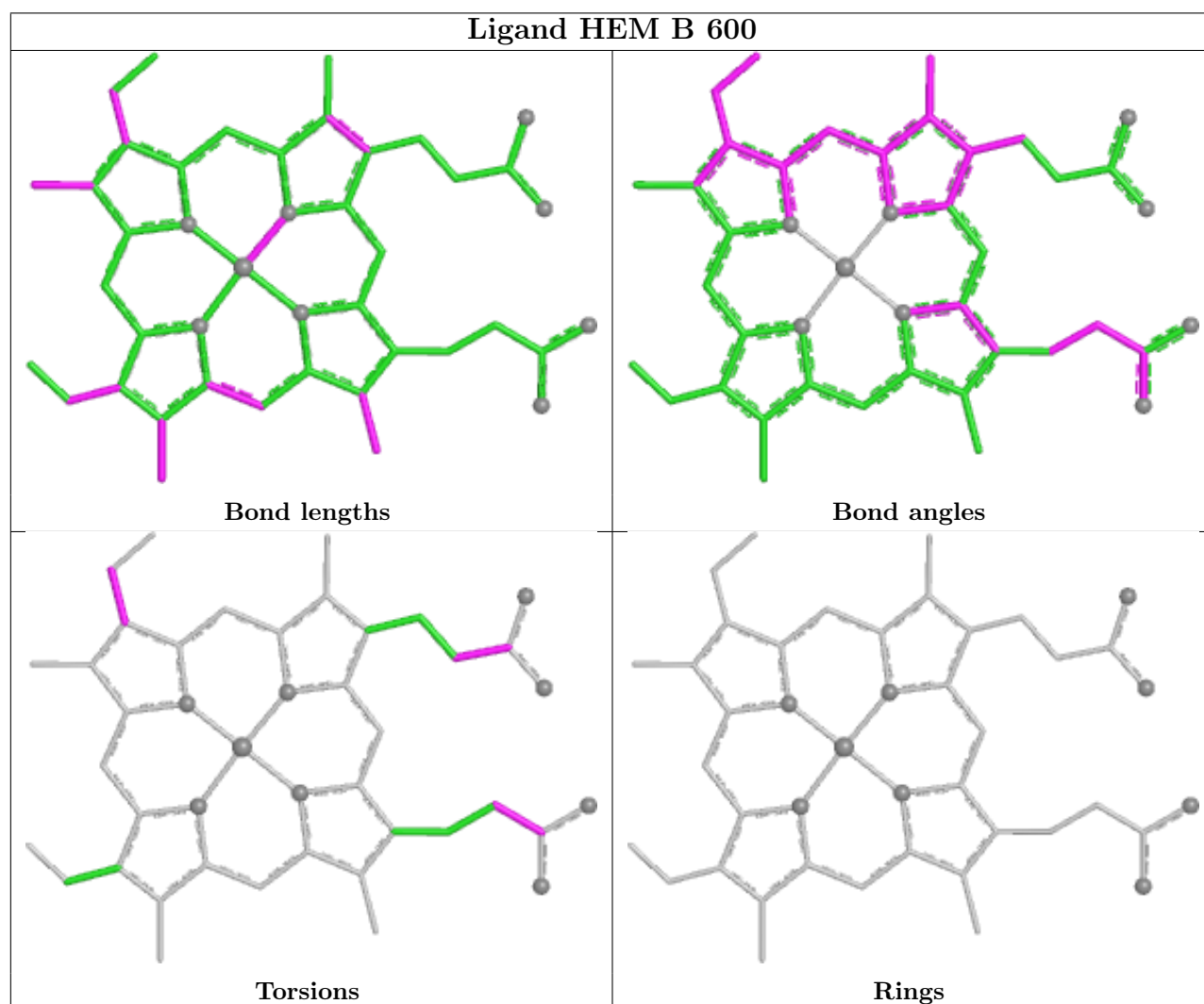
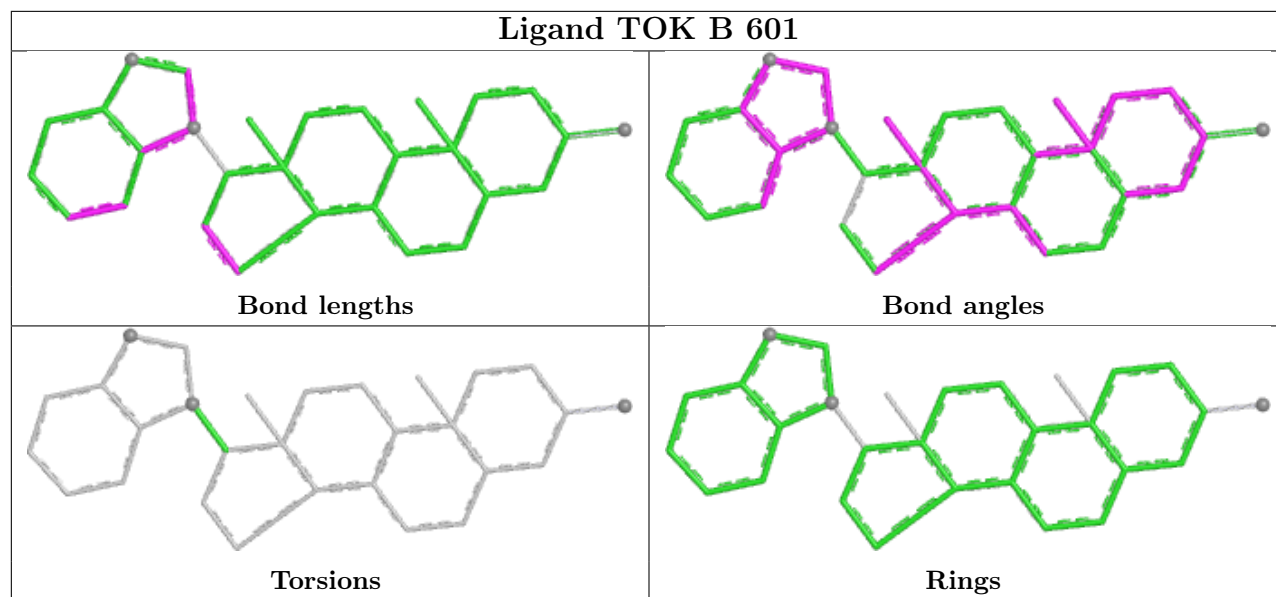
8 monomers are involved in 20 short contacts:

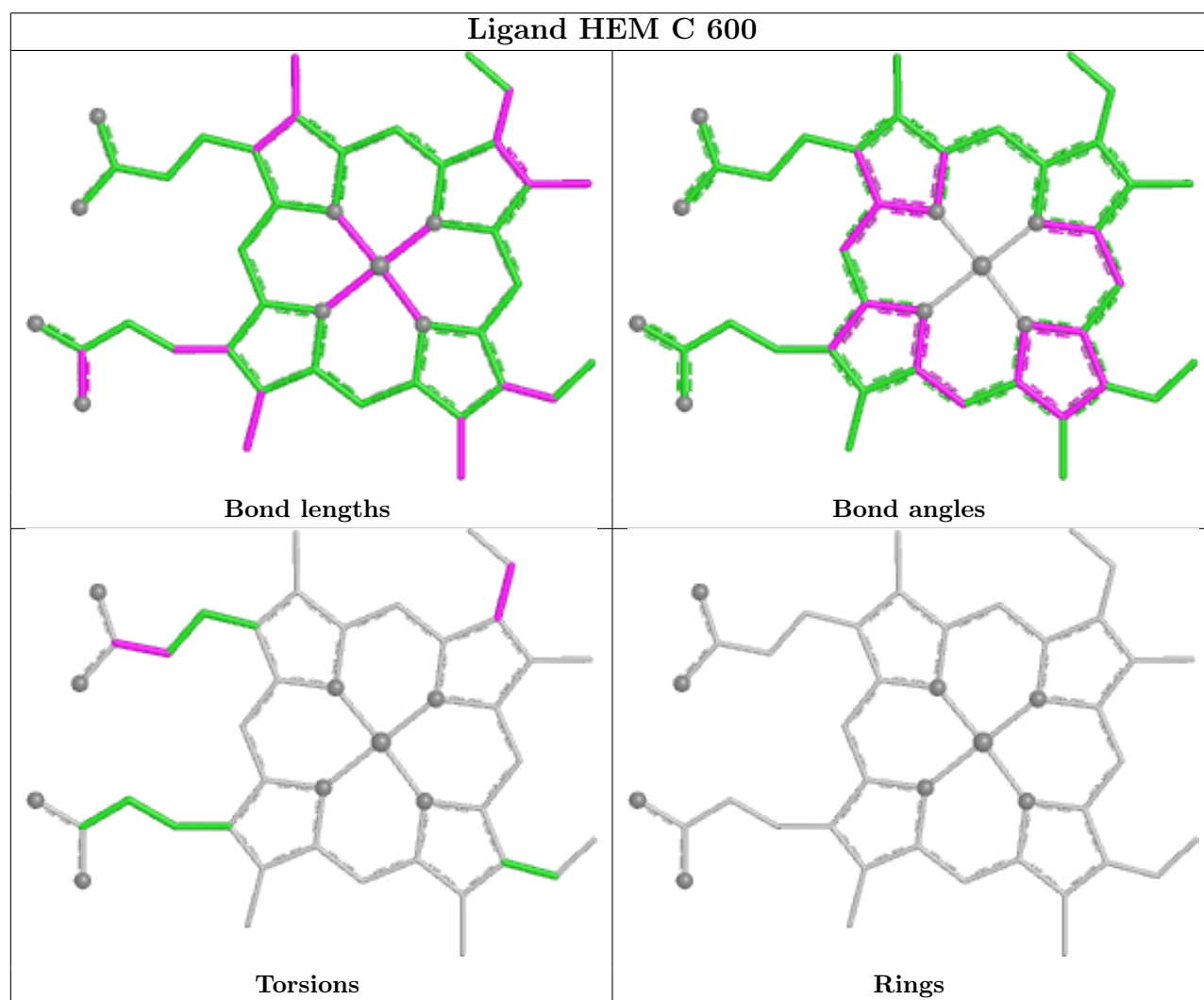
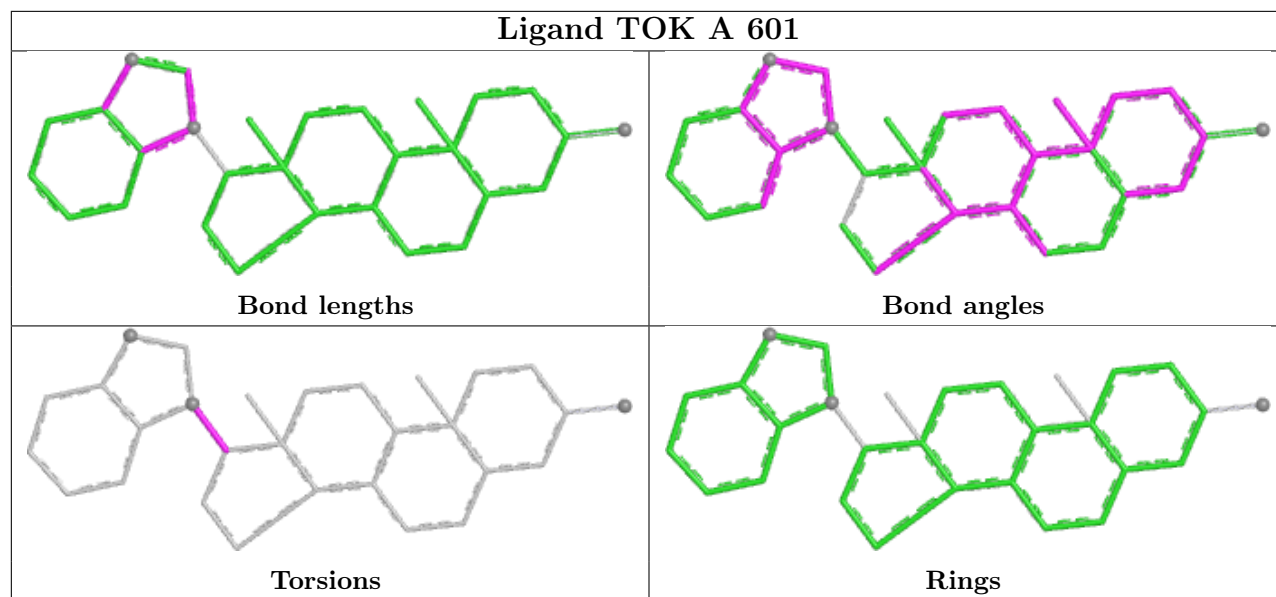
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	TOK	2	0
3	C	601	TOK	5	0
2	A	600	HEM	4	0
3	B	601	TOK	3	0
2	B	600	HEM	1	0
3	A	601	TOK	3	0
2	C	600	HEM	2	0
2	D	600	HEM	5	0

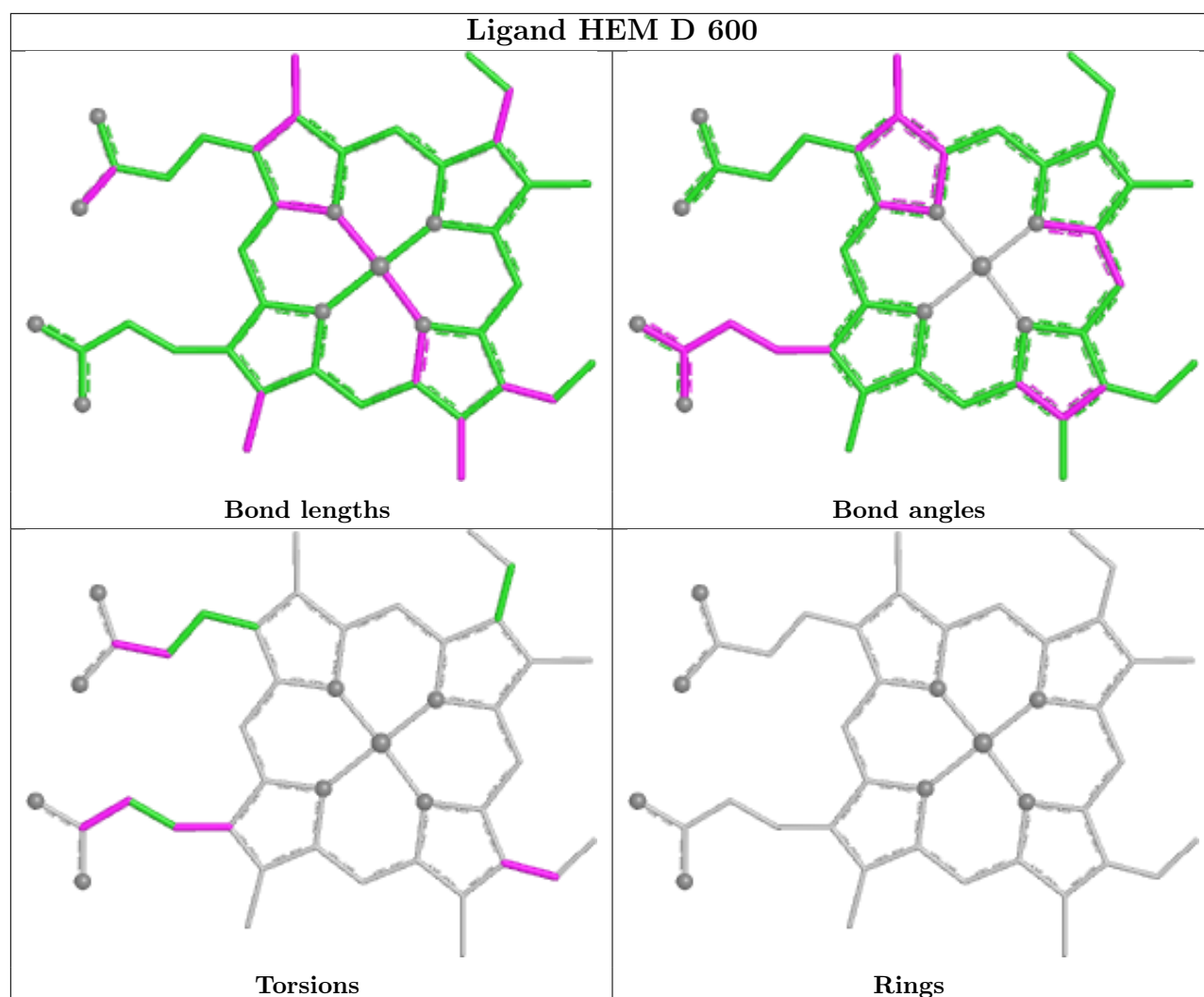
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	471/494 (95%)	0.08	8 (1%) 69 65	29, 44, 70, 81	0
1	B	465/494 (94%)	0.01	9 (1%) 66 62	25, 43, 67, 75	0
1	C	470/494 (95%)	0.12	18 (3%) 44 40	29, 43, 69, 82	1 (0%)
1	D	466/494 (94%)	0.39	20 (4%) 40 36	27, 48, 75, 87	0
All	All	1872/1976 (94%)	0.15	55 (2%) 53 50	25, 44, 71, 87	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	275	ASN	4.9
1	C	42	PHE	4.3
1	A	504	ALA	4.2
1	C	43	LEU	4.2
1	D	43	LEU	3.9
1	D	42	PHE	3.8
1	A	135	PHE	3.7
1	A	282	GLN	3.7
1	B	274	ASP	3.6
1	D	216	ASP	3.2
1	D	498	ALA	3.0
1	C	46	HIS	3.0
1	D	285	GLU	3.0
1	C	41	PRO	3.0
1	D	462	ARG	3.0
1	A	276	GLY	2.9
1	C	31	LEU	2.8
1	D	212	ASP	2.8
1	C	280	PRO	2.8
1	C	274	ASP	2.8
1	D	473	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	503	GLN	2.7
1	D	467	VAL	2.6
1	A	136	LYS	2.6
1	C	44	PRO	2.6
1	D	284	SER	2.6
1	C	276	GLY	2.5
1	B	285	GLU	2.5
1	A	283	ASP	2.4
1	D	274	ASP	2.4
1	D	162	GLY	2.4
1	D	120	HIS	2.4
1	B	134	LEU	2.4
1	C	473	LEU	2.4
1	D	337	GLY	2.3
1	C	493	ILE	2.3
1	A	139	ASP	2.3
1	C	45	ARG	2.3
1	D	41	PRO	2.3
1	D	45	ARG	2.2
1	B	138	GLY	2.2
1	B	256	SER	2.2
1	D	500	ARG	2.1
1	C	139	ASP	2.1
1	C	334[A]	GLN	2.1
1	C	471	GLY	2.1
1	B	135	PHE	2.1
1	A	275	ASN	2.1
1	C	500	ARG	2.1
1	B	470	ASP	2.1
1	C	281	ASP	2.0
1	D	140	GLN	2.0
1	D	495	VAL	2.0
1	B	156	MET	2.0
1	B	120	HIS	2.0

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

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](#)

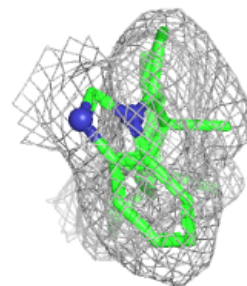
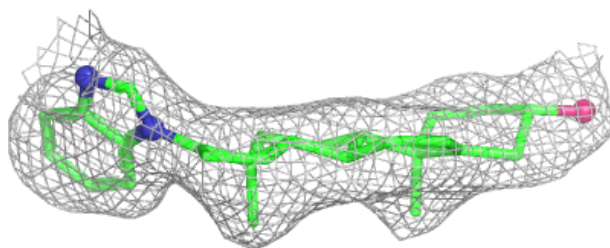
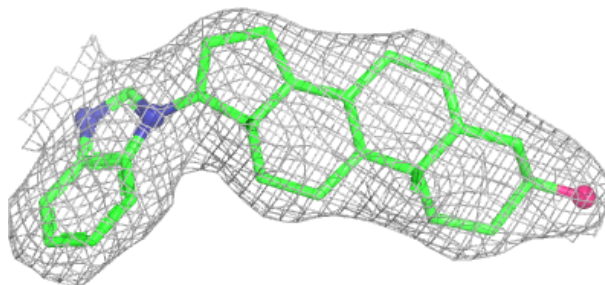
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TOK	B	601	29/29	0.94	0.08	29,35,37,40	0
3	TOK	A	601	29/29	0.95	0.08	36,41,43,44	0
3	TOK	C	601	29/29	0.95	0.08	26,31,34,35	0
3	TOK	D	601	29/29	0.95	0.07	27,32,39,43	0
2	HEM	A	600	43/43	0.97	0.09	28,36,43,47	0
2	HEM	B	600	43/43	0.97	0.07	25,33,36,40	0
2	HEM	C	600	43/43	0.98	0.07	28,34,39,41	0
2	HEM	D	600	43/43	0.98	0.07	26,30,34,36	0

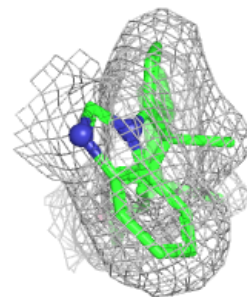
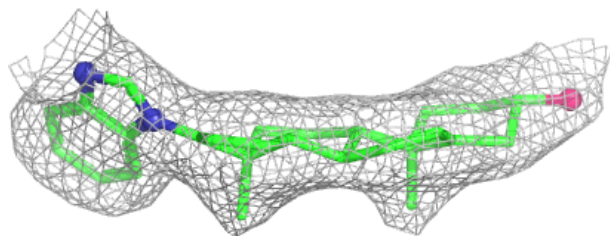
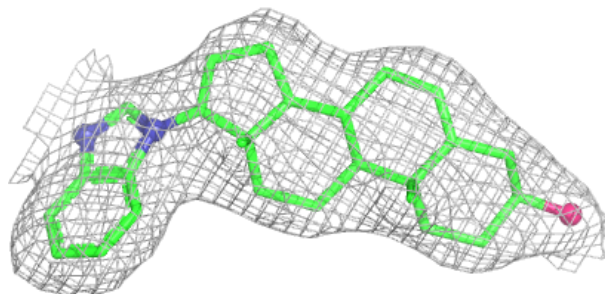
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

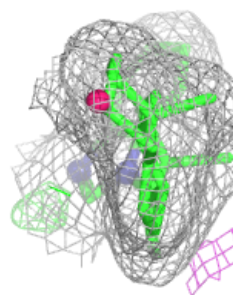
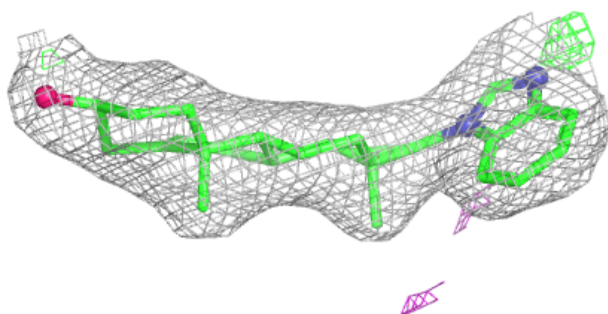
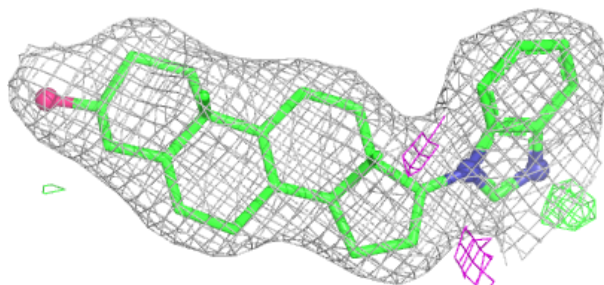
**Electron density around TOK A 601:**

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

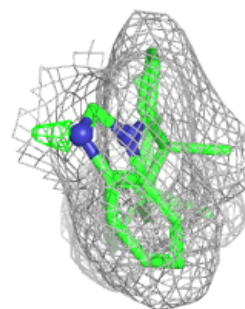
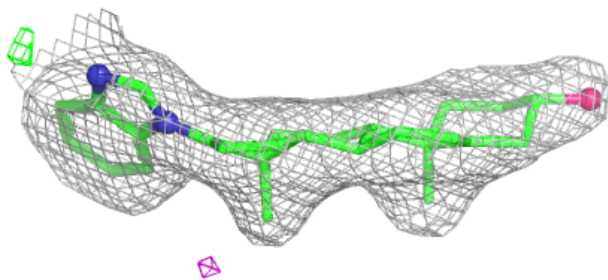
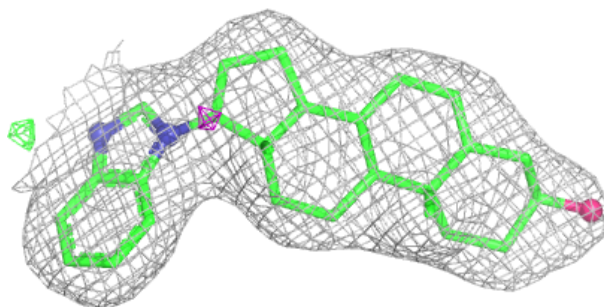


Electron density around TOK C 601:

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

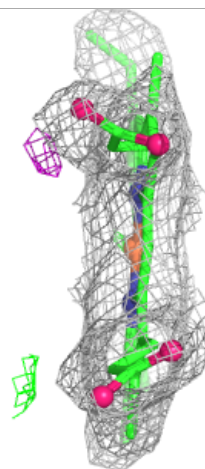
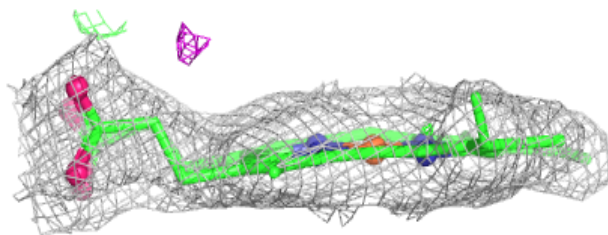
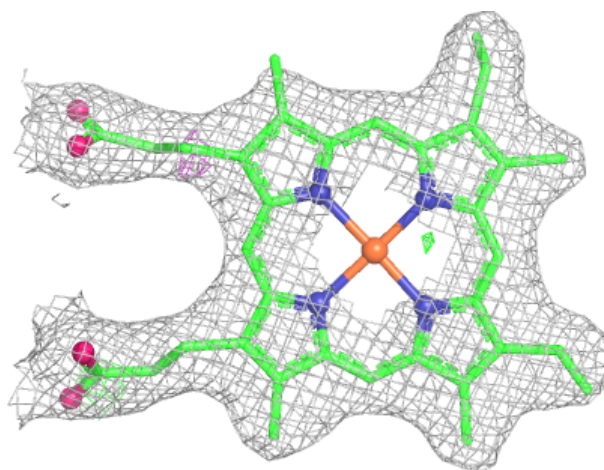
**Electron density around TOK D 601:**

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



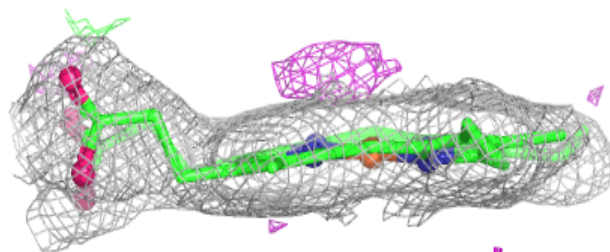
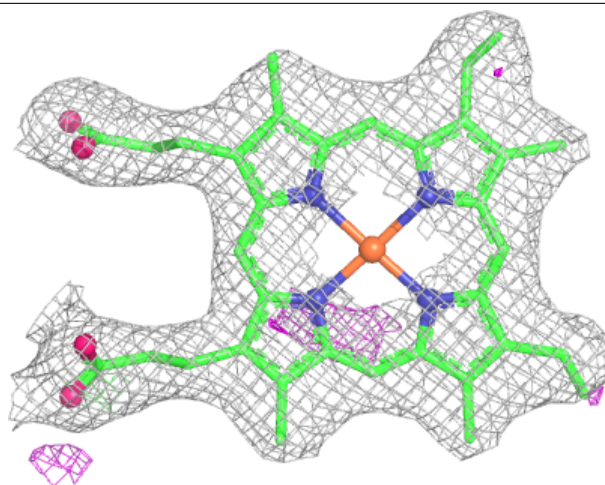
Electron density around HEM A 600:

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



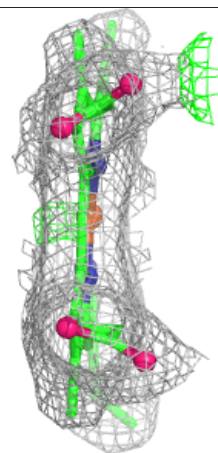
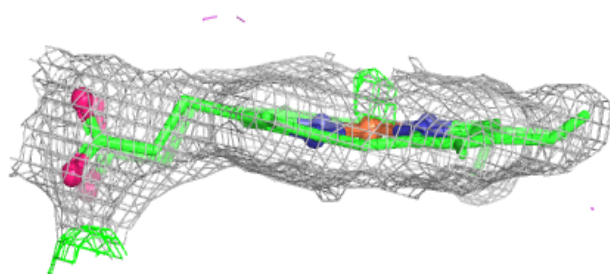
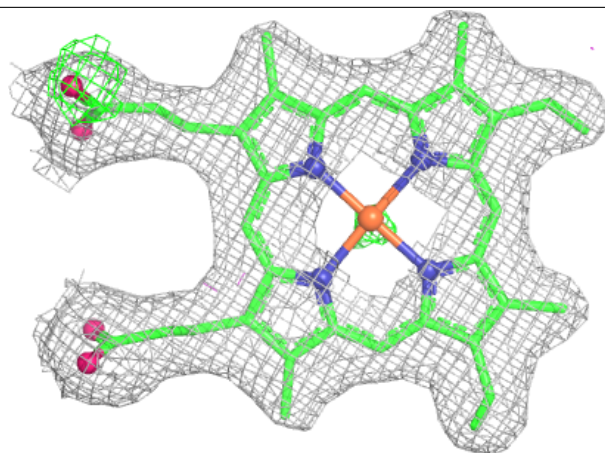
Electron density around HEM B 600:

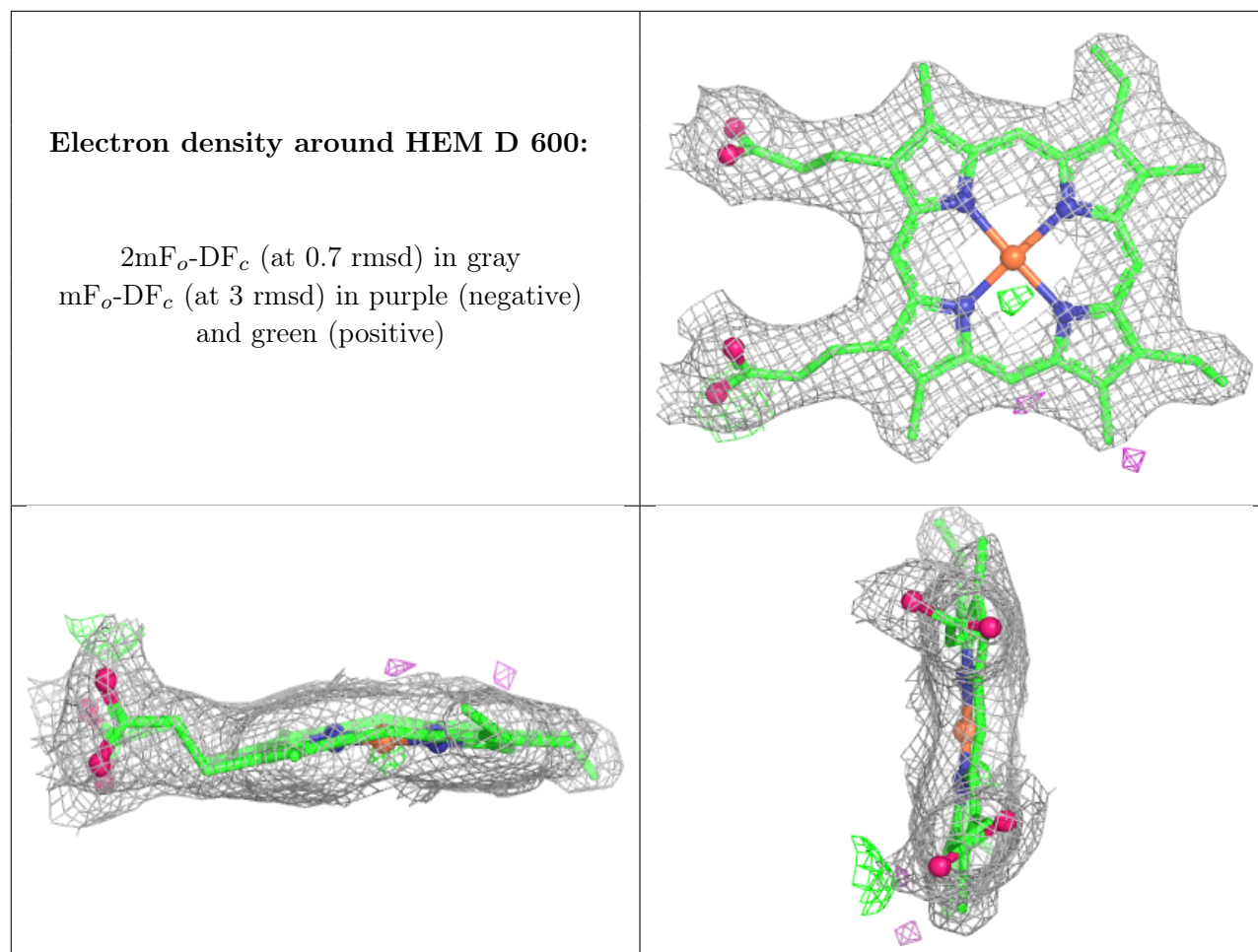
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 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.