



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:11 PM UTC

PDB ID : 4K9W / pdb_00004k9w
Title : Complex of human CYP3A4 with a desoxyritonavir analog
Authors : Sevrioukova, I.F.; Poulos, T.L.
Deposited on : 2013-04-21
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

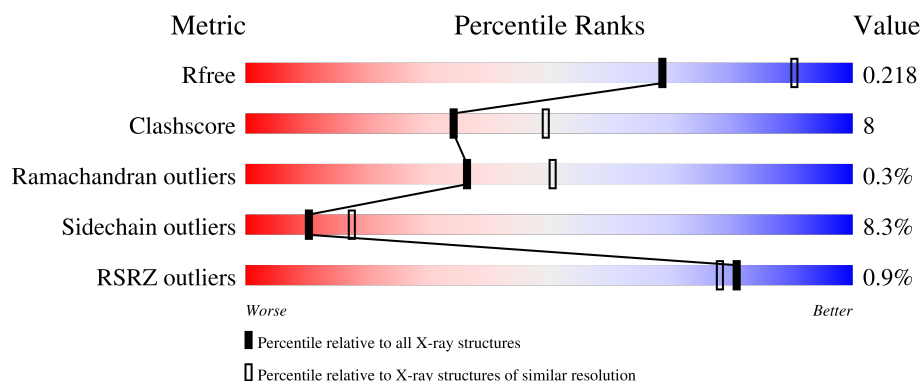
1 Overall quality at a glance

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	487	 75% 17% • 6%
1	B	487	 72% 20% • 6%
1	C	487	 75% 17% • 6%
1	D	487	 72% 19% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3687	2400	605	658	24			
1	B	457	Total	C	N	O	S	0	1	0
			3682	2397	603	658	24			
1	C	458	Total	C	N	O	S	0	0	0
			3688	2400	606	658	24			
1	D	458	Total	C	N	O	S	0	0	0
			3688	2400	606	658	24			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	UNP P08684
A	?	-	TRP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	SER	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	504	HIS	-	expression tag	UNP P08684

Continued on next page...

Continued from previous page...

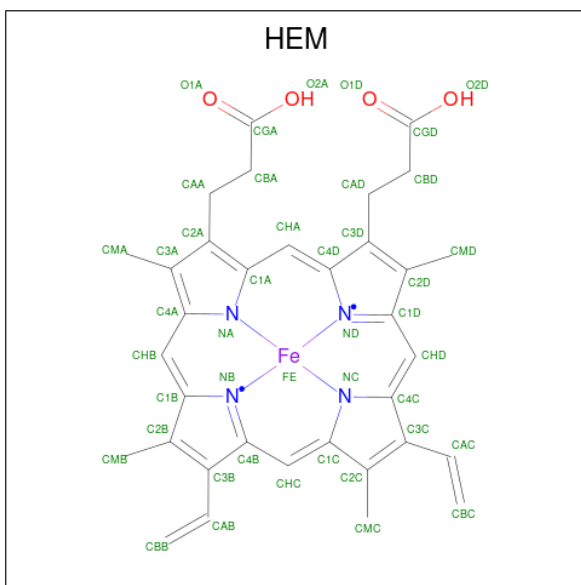
Chain	Residue	Modelled	Actual	Comment	Reference
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	GLU	deletion	UNP P08684
B	?	-	THR	deletion	UNP P08684
B	?	-	TRP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	VAL	deletion	UNP P08684
B	?	-	SER	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	VAL	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	ILE	deletion	UNP P08684
C	?	-	PRO	deletion	UNP P08684
C	?	-	ASP	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	ALA	deletion	UNP P08684
C	?	-	MET	deletion	UNP P08684
C	?	-	GLU	deletion	UNP P08684
C	?	-	THR	deletion	UNP P08684
C	?	-	TRP	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	ALA	deletion	UNP P08684
C	?	-	VAL	deletion	UNP P08684

Continued on next page...

Continued from previous page...

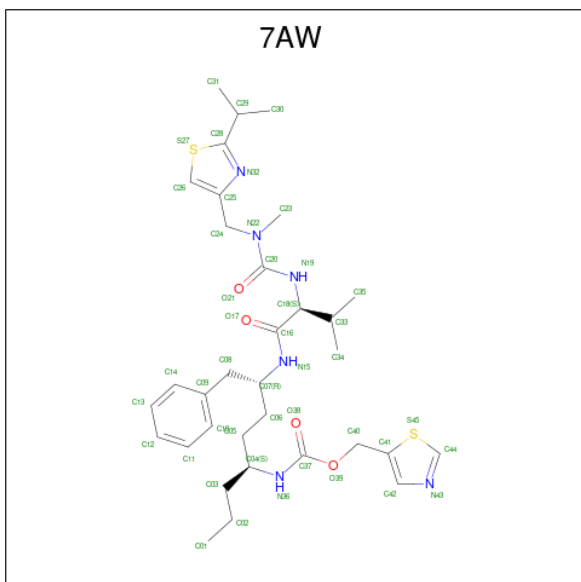
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	VAL	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	504	HIS	-	expression tag	UNP P08684
C	505	HIS	-	expression tag	UNP P08684
C	506	HIS	-	expression tag	UNP P08684
C	507	HIS	-	expression tag	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	ILE	deletion	UNP P08684
D	?	-	PRO	deletion	UNP P08684
D	?	-	ASP	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	ALA	deletion	UNP P08684
D	?	-	MET	deletion	UNP P08684
D	?	-	GLU	deletion	UNP P08684
D	?	-	THR	deletion	UNP P08684
D	?	-	TRP	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	ALA	deletion	UNP P08684
D	?	-	VAL	deletion	UNP P08684
D	?	-	SER	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	VAL	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	504	HIS	-	expression tag	UNP P08684
D	505	HIS	-	expression tag	UNP P08684
D	506	HIS	-	expression tag	UNP P08684
D	507	HIS	-	expression tag	UNP P08684

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



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

- Molecule 3 is N 2 -(methyl{[2-(propan-2-yl)-1,3-thiazol-4-yl]methyl}carbamoyl)-N-[(2R,5S)-1-phenyl-5-[[[(1,3-thiazol-5-ylmethoxy)carbonyl]amino]octan-2-yl]-L-valinamide (CCD ID: 7AW) (formula: C₃₃H₄₈N₆O₄S₂).



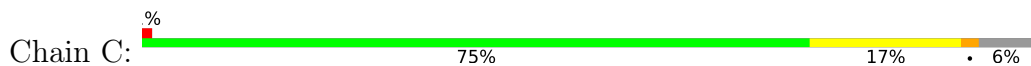
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			45	33	6	4	2		
3	B	1	Total	C	N	O	S	0	0
			45	33	6	4	2		
3	C	1	Total	C	N	O	S	0	0
			45	33	6	4	2		
3	D	1	Total	C	N	O	S	0	0
			45	33	6	4	2		

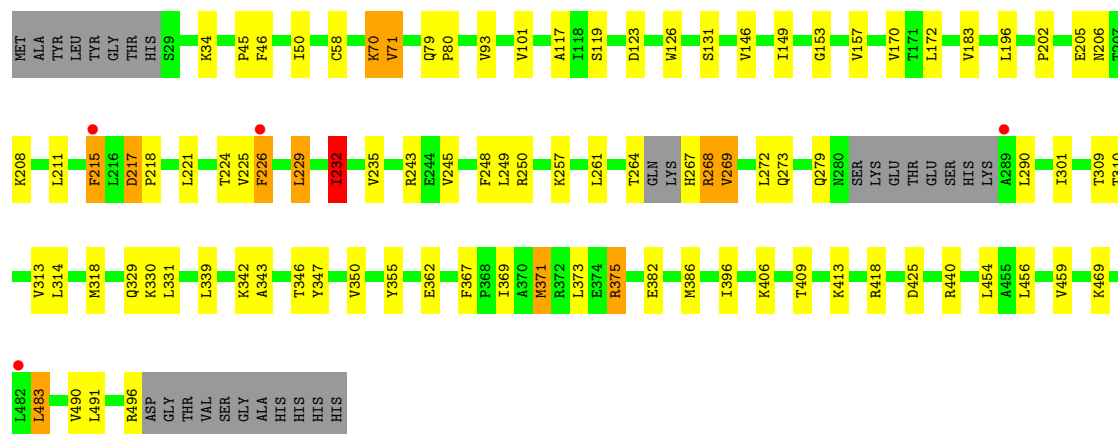
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	7	Total	O	0	0
			7	7		
4	C	7	Total	O	0	0
			7	7		
4	D	4	Total	O	0	0
			4	4		

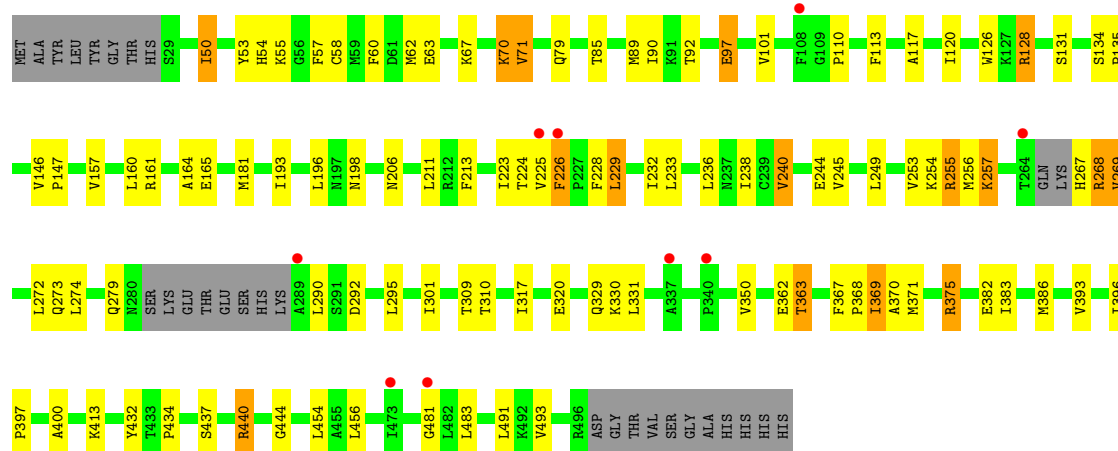
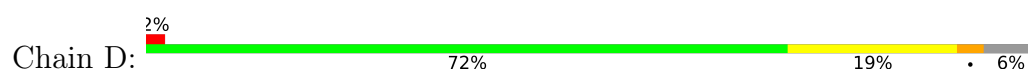
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

Chain A: 75% 17% 6%





● Molecule 1: Cytochrome P450 3A4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	94.02Å 94.02Å 199.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.01 – 2.40 47.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.01-2.40) 98.6 (47.01-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.198 0.180 , 0.218	Depositor DCC
R_{free} test set	4961 reflections (6.43%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.048 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
Reported twinning fraction	0.650 for H, K, L 0.350 for K, H, -L	Depositor
Outliers	0 of 76002 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15119	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: 7AW, 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	0.61	0/3775	0.93	6/5105 (0.1%)
1	B	0.59	0/3773	0.90	3/5104 (0.1%)
1	C	0.63	0/3777	0.92	3/5109 (0.1%)
1	D	0.64	0/3777	0.95	6/5109 (0.1%)
All	All	0.62	0/15102	0.93	18/20427 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	VAL	N-CA-C	8.72	119.80	108.12
1	D	226	PHE	CA-C-N	7.94	128.02	119.28
1	D	226	PHE	C-N-CA	7.94	128.02	119.28
1	A	86	ASP	CA-C-N	6.39	125.89	119.24
1	A	86	ASP	C-N-CA	6.39	125.89	119.24
1	A	290	LEU	N-CA-C	5.94	118.34	109.25
1	A	324	HIS	CA-C-N	5.76	126.15	119.47
1	A	324	HIS	C-N-CA	5.76	126.15	119.47
1	D	50	ILE	N-CA-C	5.67	117.08	110.62
1	C	232	ILE	CB-CA-C	-5.56	104.55	112.22
1	D	198	ASN	CA-C-N	5.43	125.08	119.05
1	D	198	ASN	C-N-CA	5.43	125.08	119.05
1	C	123	ASP	N-CA-C	5.33	116.41	108.31
1	B	201	ASP	CA-C-N	5.12	124.57	119.24
1	B	201	ASP	C-N-CA	5.12	124.57	119.24
1	C	226	PHE	N-CA-C	5.09	120.05	108.74
1	A	118	ILE	N-CA-C	5.09	115.70	110.36
1	B	211	LEU	N-CA-C	5.08	117.05	108.02

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	3687	0	3777	64	0
1	B	3682	0	3771	44	0
1	C	3688	0	3771	43	0
1	D	3688	0	3771	64	0
2	A	43	0	30	8	0
2	B	43	0	30	6	0
2	C	43	0	30	8	0
2	D	43	0	30	11	0
3	A	45	0	48	8	0
3	B	45	0	48	5	0
3	C	45	0	48	4	0
3	D	45	0	48	4	0
4	A	4	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	1	0
4	D	4	0	0	0	0
All	All	15119	0	15402	232	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 (232) 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:A:288:LYS:CB	1:A:289:ALA:HB2	1.19	1.62
1:A:288:LYS:CB	1:A:289:ALA:CB	2.06	1.32
1:A:288:LYS:HB2	1:A:289:ALA:HB2	1.10	1.08
1:D:58:CYS:SG	1:D:371:MET:HE2	1.98	1.02
1:A:288:LYS:HB3	1:A:289:ALA:CB	1.77	1.00
1:A:288:LYS:N	1:A:289:ALA:HB3	1.80	0.96
1:A:288:LYS:HB3	1:A:289:ALA:HB2	0.98	0.94
1:D:371:MET:HE3	1:D:483:LEU:HD12	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:CA	1:A:289:ALA:CB	2.46	0.92
1:A:288:LYS:HB2	1:A:289:ALA:CB	1.86	0.89
1:A:369:ILE:HG12	2:A:601:HEM:CMB	2.08	0.83
1:B:221:LEU:O	1:B:225:VAL:HG22	1.78	0.82
2:C:601:HEM:C1D	3:C:602:7AW:H4	2.15	0.81
1:A:369:ILE:HG12	2:A:601:HEM:HMB1	1.63	0.81
1:A:367:PHE:HB3	1:A:483:LEU:HD21	1.63	0.81
1:A:288:LYS:CA	1:A:289:ALA:HB2	2.09	0.80
1:D:110:PRO:HD2	1:D:240:VAL:HG13	1.64	0.80
2:A:601:HEM:ND	3:A:602:7AW:H4	2.00	0.76
1:B:71:VAL:HG21	1:B:386:MET:HE1	1.67	0.76
1:C:221:LEU:O	1:C:225:VAL:HG23	1.87	0.75
1:C:215:PHE:CZ	1:C:224:THR:HG21	2.24	0.73
1:A:134:SER:HA	1:A:443:ILE:HD11	1.69	0.73
1:C:58:CYS:SG	1:C:371:MET:HG2	2.30	0.71
2:B:601:HEM:C1D	3:B:602:7AW:H4	2.26	0.70
1:D:267:HIS:O	1:D:268:ARG:HB2	1.91	0.70
1:D:350:VAL:HG21	1:D:454:LEU:CD1	2.22	0.69
1:A:226:PHE:HB3	1:A:228:PHE:CE2	2.28	0.69
1:B:457:ILE:O	1:B:461:GLN:HG2	1.94	0.68
1:A:288:LYS:HB3	1:A:289:ALA:CA	2.23	0.67
1:A:369:ILE:CG1	2:A:601:HEM:HMB1	2.25	0.67
1:C:264:THR:O	1:C:267:HIS:NE2	2.23	0.67
1:B:369:ILE:HG12	2:B:601:HEM:HMB3	1.78	0.65
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.79	0.64
1:C:330:LYS:HD3	1:C:355:TYR:CZ	2.32	0.64
1:A:211:LEU:HD12	3:A:602:7AW:H10	1.78	0.64
1:D:90:ILE:HG23	1:D:396:ILE:HD13	1.80	0.64
1:D:375:ARG:NH2	2:D:601:HEM:O1A	2.30	0.64
2:C:601:HEM:ND	3:C:602:7AW:C42	2.61	0.64
1:B:97:GLU:HB3	1:B:101:VAL:HG13	1.79	0.63
1:A:58:CYS:SG	1:A:371:MET:HE2	2.39	0.63
1:A:331:LEU:HD12	1:A:359:VAL:HG21	1.80	0.63
1:A:422:LYS:HD2	1:C:34:LYS:HA	1.82	0.62
2:C:601:HEM:ND	3:C:602:7AW:H4	2.15	0.62
1:D:350:VAL:HG21	1:D:454:LEU:HD12	1.81	0.62
1:C:215:PHE:HZ	1:C:224:THR:HG21	1.63	0.62
1:C:172:LEU:HD11	1:C:491:LEU:HD12	1.81	0.62
1:A:446:ARG:HH11	1:B:425:ASP:HB2	1.64	0.61
1:A:288:LYS:CA	1:A:289:ALA:HB3	2.22	0.61
1:A:409:THR:O	1:A:418:ARG:NH2	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:VAL:HG13	1:D:273:GLN:HB3	1.81	0.61
1:C:71:VAL:HG21	1:C:386:MET:HE1	1.83	0.61
1:B:485:PRO:HB2	1:B:487:LYS:O	2.01	0.61
1:A:70:LYS:HA	1:A:85:THR:OG1	2.00	0.61
1:A:97:GLU:HB3	1:A:101:VAL:HG13	1.84	0.60
1:D:71:VAL:HG21	1:D:386:MET:HE1	1.83	0.60
1:D:110:PRO:O	1:D:240:VAL:HG22	2.01	0.60
2:A:601:HEM:C1D	3:A:602:7AW:H4	2.37	0.59
1:A:294:GLU:O	1:A:298:GLN:HG2	2.03	0.59
1:A:421:LYS:HA	1:A:424:LYS:HD3	1.84	0.59
1:A:383:ILE:O	1:A:383:ILE:HG13	2.03	0.59
2:B:601:HEM:ND	3:B:602:7AW:H4	2.18	0.58
1:D:368:PRO:O	1:D:483:LEU:HD13	2.03	0.58
1:B:429:PRO:O	1:B:433:THR:HG23	2.03	0.58
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.84	0.58
1:A:288:LYS:N	1:A:289:ALA:CB	2.55	0.58
1:D:126:TRP:CZ2	1:D:440:ARG:HG2	2.39	0.58
1:C:46:PHE:HD2	1:C:226:PHE:CZ	2.22	0.58
1:B:371:MET:HE3	1:B:483:LEU:HD13	1.86	0.57
1:D:236:LEU:HB2	1:D:238:ILE:HG12	1.87	0.57
1:A:184:ILE:O	1:A:188:SER:HB2	2.06	0.56
1:D:53:TYR:CD2	1:D:57:PHE:HB3	2.40	0.56
1:C:126:TRP:CZ2	1:C:440:ARG:HG2	2.42	0.55
1:B:108:PHE:CE2	1:B:120:ILE:HG12	2.42	0.55
1:A:117:ALA:HB1	1:A:301:ILE:CG1	2.38	0.54
1:D:161:ARG:O	1:D:165:GLU:HG2	2.07	0.54
1:C:369:ILE:HG12	2:C:601:HEM:CMB	2.37	0.54
2:B:601:HEM:ND	3:B:602:7AW:C42	2.71	0.54
1:D:309:THR:HG22	2:D:601:HEM:HAB	1.89	0.54
1:B:108:PHE:HE2	1:B:120:ILE:HG12	1.73	0.54
1:B:356:LEU:O	1:B:360:VAL:HG23	2.07	0.54
1:A:461:GLN:HA	1:A:496:ARG:HH21	1.73	0.53
1:A:226:PHE:HB3	1:A:228:PHE:HE2	1.73	0.53
1:C:225:VAL:HG12	1:C:226:PHE:CG	2.43	0.53
1:A:235:VAL:C	1:A:237:ASN:H	2.17	0.52
1:D:317:ILE:HA	1:D:363:THR:HG21	1.91	0.52
1:B:225:VAL:HG23	1:B:226:PHE:CD1	2.44	0.52
1:B:356:LEU:HD21	1:B:453:LYS:HB3	1.92	0.52
1:D:160:LEU:HD22	1:D:493:VAL:HG21	1.92	0.52
2:D:601:HEM:C1D	3:D:602:7AW:H4	2.45	0.52
3:A:602:7AW:H5	3:A:602:7AW:H18	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:PRO:HB2	1:D:274:LEU:HD21	1.92	0.51
1:D:253:VAL:HA	1:D:256:MET:HE3	1.92	0.51
1:C:375:ARG:NH2	2:C:601:HEM:O1A	2.39	0.51
2:C:601:HEM:NB	3:C:602:7AW:H3	2.25	0.51
1:D:375:ARG:HH22	2:D:601:HEM:CGA	2.23	0.51
2:D:601:HEM:ND	3:D:602:7AW:H4	2.25	0.51
1:D:53:TYR:CE2	1:D:57:PHE:HB3	2.46	0.50
1:D:257:LYS:NZ	1:D:292:ASP:OD2	2.44	0.50
2:A:601:HEM:ND	3:A:602:7AW:C42	2.69	0.50
1:C:269:VAL:HG13	1:C:273:GLN:CG	2.41	0.50
1:B:375:ARG:NH2	2:B:601:HEM:O1A	2.45	0.50
1:C:202:PRO:HB2	1:C:248:PHE:CZ	2.47	0.50
1:A:143:LYS:HE3	1:A:347:TYR:CD1	2.47	0.50
1:C:267:HIS:O	1:C:268:ARG:HB3	2.11	0.50
1:C:269:VAL:HG13	1:C:273:GLN:HG3	1.94	0.49
2:A:601:HEM:C4D	3:A:602:7AW:H4	2.46	0.49
1:C:369:ILE:HG12	2:C:601:HEM:HMB1	1.94	0.49
1:D:58:CYS:HG	1:D:371:MET:HE2	1.75	0.49
1:D:367:PHE:HB3	1:D:483:LEU:HD21	1.93	0.49
1:C:117:ALA:HB1	1:C:301:ILE:CG1	2.43	0.48
1:D:255:ARG:HH11	1:D:255:ARG:HB2	1.78	0.48
1:B:369:ILE:CG1	2:B:601:HEM:HMB3	2.43	0.48
1:C:153:GLY:O	1:C:157:VAL:HG22	2.14	0.48
1:D:213:PHE:CD2	1:D:481:GLY:HA3	2.49	0.48
1:B:251:LYS:HG2	1:B:255:ARG:HH21	1.79	0.48
1:C:206:ASN:HB3	1:C:245:VAL:HG13	1.96	0.48
1:A:111:VAL:O	1:A:114:MET:HB2	2.14	0.48
1:C:146:VAL:HG21	1:C:347:TYR:HB2	1.96	0.47
1:D:223:ILE:HG13	1:D:224:THR:N	2.29	0.47
1:A:89:MET:O	1:A:93:VAL:HG13	2.15	0.47
1:B:257:LYS:NZ	1:B:292:ASP:OD2	2.47	0.47
1:D:350:VAL:HG21	1:D:454:LEU:HD11	1.95	0.47
1:D:362:GLU:OE2	1:D:362:GLU:HA	2.14	0.47
1:C:172:LEU:HD11	1:C:491:LEU:CD1	2.43	0.47
1:D:229:LEU:HD12	1:D:232:ILE:HD12	1.96	0.47
1:D:54:HIS:CE1	1:D:55:LYS:HG2	2.49	0.47
1:D:320:GLU:OE2	1:D:320:GLU:HA	2.15	0.46
1:B:106:ARG:NH2	1:B:374:GLU:OE1	2.26	0.46
1:B:202:PRO:HB2	1:B:248:PHE:CZ	2.50	0.46
1:D:117:ALA:HB3	1:D:120:ILE:HD12	1.96	0.46
1:D:233:LEU:HB3	1:D:238:ILE:HB	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:N	1:A:135:PRO:CD	2.77	0.46
1:A:356:LEU:O	1:A:360:VAL:HG23	2.15	0.46
1:B:189:PHE:HD2	1:B:272:LEU:HG	1.80	0.46
1:A:134:SER:CA	1:A:443:ILE:HD11	2.40	0.46
1:A:141:LYS:O	1:A:145:MET:HG3	2.16	0.46
1:B:76:ASP:OD2	1:B:106:ARG:NH1	2.47	0.46
1:C:243:ARG:NH1	4:C:707:HOH:O	2.48	0.46
1:B:250:ARG:HG3	1:B:296:VAL:HG11	1.98	0.45
1:A:331:LEU:HD22	1:A:460:LEU:HD13	1.98	0.45
1:B:154:ASP:OD2	1:B:458:ARG:NH2	2.48	0.45
1:A:135:PRO:O	1:A:141:LYS:NZ	2.49	0.45
1:D:432:TYR:CZ	1:D:434:PRO:HG3	2.52	0.45
1:D:223:ILE:C	1:D:225:VAL:H	2.23	0.45
1:C:79:GLN:NE2	1:C:80:PRO:HD2	2.32	0.45
1:C:170:VAL:O	1:C:490:VAL:HA	2.17	0.45
1:C:346:THR:O	1:C:350:VAL:HG23	2.16	0.45
1:C:339:LEU:HB3	1:C:343:ALA:HB3	1.99	0.45
1:D:70:LYS:HA	1:D:85:THR:OG1	2.17	0.45
1:A:331:LEU:HD21	1:A:356:LEU:HD13	1.98	0.45
1:A:349:THR:O	1:A:353:MET:HG3	2.17	0.45
1:B:233:LEU:HB3	1:B:238:ILE:HB	1.99	0.45
1:A:350:VAL:HG21	1:A:454:LEU:HD13	1.99	0.44
3:D:602:7AW:C26	3:D:602:7AW:H34	2.47	0.44
1:B:467:PRO:HB3	1:B:473:ILE:HD11	2.00	0.44
1:C:373:LEU:HB2	1:C:396:ILE:HB	2.00	0.44
1:D:397:PRO:HB2	1:D:400:ALA:HB3	1.99	0.44
1:A:126:TRP:CZ2	1:A:440:ARG:HG2	2.52	0.44
1:D:79:GLN:NE2	1:D:393:VAL:HG23	2.32	0.44
1:A:154:ASP:OD2	1:A:458:ARG:NH2	2.51	0.44
1:A:201:ASP:HA	1:A:202:PRO:HD2	1.87	0.44
1:A:257:LYS:NZ	1:A:292:ASP:OD2	2.48	0.43
1:B:253:VAL:HA	1:B:256:MET:HE3	2.00	0.43
3:B:602:7AW:N36	3:B:602:7AW:H18	2.33	0.43
1:D:369:ILE:HG13	1:D:370:ALA:H	1.83	0.43
1:A:369:ILE:HD11	2:A:601:HEM:CHB	2.49	0.43
3:B:602:7AW:H37	3:B:602:7AW:H20	2.00	0.43
1:C:309:THR:O	1:C:313:VAL:HG23	2.18	0.43
1:A:78:GLN:O	1:A:80:PRO:HD3	2.19	0.43
1:A:235:VAL:C	1:A:237:ASN:N	2.75	0.43
1:B:91:LYS:HE3	1:B:96:LYS:HE3	2.00	0.43
1:B:230:ILE:HB	1:B:231:PRO:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HB2	1:A:248:PHE:CZ	2.54	0.43
1:B:163:GLU:H	1:B:163:GLU:HG2	1.70	0.43
1:C:70:LYS:HE2	1:C:70:LYS:HB2	1.90	0.43
1:D:63:GLU:O	1:D:67:LYS:HB2	2.18	0.43
1:D:369:ILE:HG12	2:D:601:HEM:CMB	2.49	0.43
1:A:158:ARG:NH2	1:A:197:ASN:OD1	2.50	0.43
1:C:217:ASP:HA	1:C:218:PRO:HD3	1.90	0.43
1:A:301:ILE:HD12	3:A:602:7AW:O38	2.19	0.42
1:D:92:THR:HG22	1:D:97:GLU:HG3	2.01	0.42
1:B:279:GLN:HG2	1:B:290:LEU:O	2.18	0.42
2:D:601:HEM:ND	3:D:602:7AW:C42	2.81	0.42
1:B:319:TYR:CZ	1:B:475:LEU:HB2	2.54	0.42
1:D:117:ALA:HB1	1:D:301:ILE:HG13	2.01	0.42
1:D:57:PHE:HA	1:D:60:PHE:HB3	2.02	0.42
1:B:168:LYS:HA	1:B:169:PRO:HD2	1.88	0.42
1:B:90:ILE:HG12	1:B:396:ILE:HG12	2.00	0.42
1:B:135:PRO:HB2	1:B:274:LEU:HD21	2.00	0.42
1:D:257:LYS:HE3	1:D:295:LEU:HD13	2.02	0.42
1:C:314:LEU:O	1:C:318:MET:HG2	2.20	0.42
1:D:90:ILE:HG23	1:D:396:ILE:CD1	2.49	0.42
1:D:279:GLN:HG2	1:D:290:LEU:O	2.20	0.42
1:A:461:GLN:HA	1:A:496:ARG:NH2	2.34	0.42
1:B:117:ALA:HB1	1:B:301:ILE:HG13	2.02	0.42
1:B:179:TYR:CZ	1:B:455:ALA:HB2	2.55	0.42
1:C:369:ILE:CG1	2:C:601:HEM:HMB1	2.50	0.42
1:D:89:MET:HG3	1:D:383:ILE:HD12	2.02	0.42
1:D:164:ALA:HB2	1:D:493:VAL:HG12	2.02	0.41
1:D:224:THR:O	1:D:224:THR:HG22	2.20	0.41
1:D:309:THR:CG2	2:D:601:HEM:HAB	2.50	0.41
3:A:602:7AW:O38	3:A:602:7AW:H8	2.21	0.41
1:B:219:PHE:O	1:B:223:ILE:HG12	2.20	0.41
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.85	0.41
1:C:149:ILE:HG12	1:C:183:VAL:HG13	2.02	0.41
1:D:128:ARG:H	1:D:128:ARG:HG2	1.65	0.41
1:D:146:VAL:HB	1:D:147:PRO:HD3	2.01	0.41
1:B:299:SER:O	1:B:300:ILE:C	2.63	0.41
1:A:130:ARG:O	1:A:134:SER:HB3	2.20	0.41
1:D:226:PHE:HB3	1:D:228:PHE:CE2	2.55	0.41
1:A:225:VAL:O	1:A:227:PRO:HD3	2.21	0.41
1:C:225:VAL:HG12	1:C:226:PHE:CD1	2.56	0.41
1:D:206:ASN:HB3	1:D:245:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:HB3	1:B:228:PHE:CZ	2.56	0.41
1:D:444:GLY:HA3	2:D:601:HEM:C3C	2.55	0.41
1:A:102:PHE:O	1:A:375:ARG:HD3	2.21	0.41
1:B:70:LYS:HE2	1:B:70:LYS:HB2	1.95	0.41
1:C:45:PRO:O	1:C:46:PHE:HB2	2.21	0.41
1:D:413:LYS:HA	1:D:413:LYS:HD3	1.79	0.41
1:A:161:ARG:O	1:A:165:GLU:HG2	2.21	0.41
1:C:362:GLU:HA	1:C:362:GLU:OE2	2.21	0.41
1:D:181:MET:HG3	1:D:193:ILE:HD11	2.03	0.41
1:A:233:LEU:HA	1:A:236:LEU:HD12	2.04	0.40
1:C:279:GLN:HG2	1:C:290:LEU:O	2.21	0.40
1:C:330:LYS:HD3	1:C:355:TYR:CE2	2.56	0.40
1:D:309:THR:HG22	2:D:601:HEM:CAB	2.49	0.40
1:D:309:THR:HG21	2:D:601:HEM:C3B	2.56	0.40
1:C:367:PHE:HB3	1:C:483:LEU:HD21	2.03	0.40
1:D:113:PHE:CD2	1:D:113:PHE:C	3.00	0.40
1:C:229:LEU:HD12	1:C:232:ILE:HD11	2.01	0.40
1:B:202:PRO:HB2	1:B:248:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/487 (93%)	431 (95%)	18 (4%)	3 (1%)	18	28
1	B	452/487 (93%)	435 (96%)	16 (4%)	1 (0%)	43	58
1	C	452/487 (93%)	429 (95%)	22 (5%)	1 (0%)	43	58
1	D	452/487 (93%)	428 (95%)	23 (5%)	1 (0%)	43	58
All	All	1808/1948 (93%)	1723 (95%)	79 (4%)	6 (0%)	36	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ALA
1	A	236	LEU
1	A	421	LYS
1	C	268	ARG
1	D	268	ARG
1	B	481	GLY

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	419/443 (95%)	392 (94%)	27 (6%)	16	28
1	B	419/443 (95%)	379 (90%)	40 (10%)	8	13
1	C	419/443 (95%)	379 (90%)	40 (10%)	8	13
1	D	419/443 (95%)	387 (92%)	32 (8%)	12	21
All	All	1676/1772 (95%)	1537 (92%)	139 (8%)	10	17

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	70	LYS
1	A	71	VAL
1	A	88	ASP
1	A	89	MET
1	A	93	VAL
1	A	101	VAL
1	A	103	THR
1	A	115	LYS
1	A	168	LYS
1	A	191	VAL
1	A	196	LEU
1	A	205	GLU
1	A	208	LYS
1	A	211	LEU
1	A	229	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	249	LEU
1	A	272	LEU
1	A	274	LEU
1	A	280	ASN
1	A	288	LYS
1	A	342	LYS
1	A	421	LYS
1	A	424	LYS
1	A	454	LEU
1	A	456	LEU
1	A	484	GLN
1	B	30	HIS
1	B	34	LYS
1	B	36	LEU
1	B	42	THR
1	B	55	LYS
1	B	70	LYS
1	B	78	GLN
1	B	89	MET
1	B	93	VAL
1	B	101	VAL
1	B	111	VAL
1	B	115	LYS
1	B	125	GLU
1	B	128	ARG
1	B	157	VAL
1	B	163	GLU
1	B	168	LYS
1	B	196	LEU
1	B	201	ASP
1	B	229	LEU
1	B	244	GLU
1	B	249	LEU
1	B	259	SER
1	B	264	THR
1	B	272	LEU
1	B	274	LEU
1	B	330	LYS
1	B	331	LEU
1	B	342	LYS
1	B	350	VAL
1	B	371	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	375	ARG
1	B	382	GLU
1	B	433	THR
1	B	443	ILE
1	B	454	LEU
1	B	456	LEU
1	B	469	LYS
1	B	495	SER
1	B	496	ARG
1	C	50	ILE
1	C	70	LYS
1	C	71	VAL
1	C	93	VAL
1	C	101	VAL
1	C	119	SER
1	C	131	SER
1	C	196	LEU
1	C	205	GLU
1	C	208	LYS
1	C	211	LEU
1	C	215	PHE
1	C	217	ASP
1	C	229	LEU
1	C	232	ILE
1	C	235	VAL
1	C	249	LEU
1	C	250	ARG
1	C	257	LYS
1	C	261	LEU
1	C	269	VAL
1	C	272	LEU
1	C	310	THR
1	C	329	GLN
1	C	331	LEU
1	C	342	LYS
1	C	371	MET
1	C	375	ARG
1	C	382	GLU
1	C	406	LYS
1	C	409	THR
1	C	413	LYS
1	C	418	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	425	ASP
1	C	454	LEU
1	C	456	LEU
1	C	459	VAL
1	C	469	LYS
1	C	483	LEU
1	C	496	ARG
1	D	50	ILE
1	D	62	MET
1	D	70	LYS
1	D	71	VAL
1	D	97	GLU
1	D	101	VAL
1	D	128	ARG
1	D	131	SER
1	D	134	SER
1	D	157	VAL
1	D	196	LEU
1	D	211	LEU
1	D	229	LEU
1	D	240	VAL
1	D	244	GLU
1	D	249	LEU
1	D	254	LYS
1	D	255	ARG
1	D	257	LYS
1	D	272	LEU
1	D	310	THR
1	D	329	GLN
1	D	330	LYS
1	D	331	LEU
1	D	363	THR
1	D	369	ILE
1	D	375	ARG
1	D	382	GLU
1	D	437	SER
1	D	440	ARG
1	D	456	LEU
1	D	491	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	341	ASN
1	A	426	ASN
1	A	461	GLN
1	A	472	GLN
1	B	237	ASN
1	B	280	ASN
1	B	324	HIS
1	B	329	GLN
1	B	332	GLN
1	B	352	GLN
1	B	423	ASN
1	B	451	ASN
1	B	461	GLN
1	B	472	GLN
1	C	54	HIS
1	C	79	GLN
1	C	192	ASN
1	C	237	ASN
1	C	352	GLN
1	C	472	GLN
1	D	197	ASN
1	D	237	ASN
1	D	332	GLN
1	D	352	GLN
1	D	384	ASN
1	D	451	ASN
1	D	461	GLN

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
2	HEM	B	601	1,3	50,50,50	2.66	22 (44%)	67,82,82	3.07	33 (49%)
3	7AW	C	602	2	46,47,47	1.05	3 (6%)	52,62,62	1.87	14 (26%)
3	7AW	A	602	2	46,47,47	1.12	3 (6%)	52,62,62	2.02	14 (26%)
3	7AW	B	602	2	46,47,47	1.06	3 (6%)	52,62,62	1.79	10 (19%)
3	7AW	D	602	2	46,47,47	1.06	3 (6%)	52,62,62	1.85	13 (25%)
2	HEM	D	601	1,3	50,50,50	2.62	23 (46%)	67,82,82	3.15	33 (49%)
2	HEM	C	601	1,3	50,50,50	2.75	25 (50%)	67,82,82	3.06	30 (44%)
2	HEM	A	601	1,3	50,50,50	2.60	24 (48%)	67,82,82	2.98	28 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	601	1,3	-	5/14/54/54	-
3	7AW	C	602	2	-	23/49/49/49	0/3/3/3
3	7AW	A	602	2	-	22/49/49/49	0/3/3/3
3	7AW	B	602	2	-	19/49/49/49	0/3/3/3
3	7AW	D	602	2	-	22/49/49/49	0/3/3/3
2	HEM	D	601	1,3	-	4/14/54/54	-
2	HEM	C	601	1,3	-	4/14/54/54	-
2	HEM	A	601	1,3	-	2/14/54/54	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	FE-NB	6.52	2.15	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	FE-NB	6.45	2.14	1.94
2	B	601	HEM	FE-ND	5.95	2.13	1.94
2	A	601	HEM	FE-NB	5.82	2.12	1.94
2	B	601	HEM	FE-NB	5.80	2.12	1.94
2	C	601	HEM	FE-ND	5.79	2.12	1.94
2	A	601	HEM	FE-ND	5.07	2.10	1.94
3	A	602	7AW	O39-C37	5.06	1.45	1.35
2	B	601	HEM	C3C-C2C	4.99	1.47	1.37
3	B	602	7AW	O39-C37	4.96	1.45	1.35
2	D	601	HEM	C3C-C2C	4.88	1.47	1.37
3	C	602	7AW	O39-C37	4.86	1.44	1.35
2	B	601	HEM	C3B-C2B	4.82	1.46	1.37
2	A	601	HEM	C3C-C2C	4.79	1.46	1.37
2	A	601	HEM	C3D-C2D	4.76	1.47	1.36
2	D	601	HEM	FE-ND	4.74	2.09	1.94
2	B	601	HEM	C1C-NC	4.69	1.48	1.39
2	C	601	HEM	C3D-C2D	4.61	1.46	1.36
2	B	601	HEM	C3D-C2D	4.59	1.46	1.36
3	D	602	7AW	O39-C37	4.59	1.44	1.35
2	C	601	HEM	C3C-C2C	4.45	1.46	1.37
2	C	601	HEM	C1C-NC	4.41	1.47	1.39
2	C	601	HEM	C1A-NA	4.40	1.47	1.39
2	C	601	HEM	C3B-C2B	4.37	1.46	1.37
2	D	601	HEM	C3D-C2D	4.33	1.46	1.36
2	C	601	HEM	CHD-C4C	4.33	1.46	1.38
2	D	601	HEM	C3B-C2B	4.31	1.45	1.37
2	D	601	HEM	C1C-NC	4.22	1.47	1.39
2	D	601	HEM	C1A-NA	4.21	1.47	1.39
2	A	601	HEM	CHD-C4C	4.19	1.46	1.38
2	A	601	HEM	C3B-C2B	4.14	1.45	1.37
2	D	601	HEM	CHC-C1C	4.09	1.46	1.38
2	D	601	HEM	CHD-C4C	4.05	1.46	1.38
2	C	601	HEM	CHA-C4D	4.03	1.46	1.38
2	B	601	HEM	CHD-C4C	3.98	1.46	1.38
2	C	601	HEM	C4A-NA	3.94	1.47	1.39
2	D	601	HEM	CHA-C4D	3.94	1.46	1.38
2	A	601	HEM	C4A-NA	3.81	1.46	1.39
2	C	601	HEM	CHB-C4A	3.80	1.47	1.39
2	B	601	HEM	CHA-C4D	3.76	1.46	1.38
2	A	601	HEM	C4C-NC	3.69	1.46	1.39
2	B	601	HEM	CHC-C1C	3.67	1.45	1.38
2	A	601	HEM	C1C-NC	3.67	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C2A-C3A	3.60	1.48	1.38
2	B	601	HEM	C4A-NA	3.58	1.46	1.39
2	C	601	HEM	CHC-C1C	3.57	1.45	1.38
2	A	601	HEM	C4D-ND	-3.55	1.34	1.40
2	B	601	HEM	C1A-NA	3.53	1.46	1.39
2	D	601	HEM	C4C-NC	3.50	1.46	1.39
2	D	601	HEM	C4D-ND	-3.48	1.34	1.40
2	A	601	HEM	C1A-NA	3.47	1.46	1.39
2	C	601	HEM	C4D-ND	-3.45	1.34	1.40
2	B	601	HEM	C4C-NC	3.42	1.46	1.39
2	C	601	HEM	CHA-C1A	3.39	1.47	1.39
2	A	601	HEM	CHD-C1D	3.36	1.46	1.39
2	A	601	HEM	CHA-C4D	3.34	1.45	1.38
2	D	601	HEM	CHC-C4B	3.31	1.46	1.39
2	D	601	HEM	C4A-NA	3.29	1.45	1.39
2	C	601	HEM	CHB-C1B	3.29	1.45	1.38
2	C	601	HEM	CHC-C4B	3.27	1.46	1.39
2	C	601	HEM	CHD-C1D	3.21	1.46	1.39
2	B	601	HEM	C2A-C3A	3.15	1.47	1.38
2	A	601	HEM	CHC-C1C	3.13	1.44	1.38
2	C	601	HEM	C4C-NC	3.12	1.45	1.39
2	B	601	HEM	CHC-C4B	3.09	1.46	1.39
2	D	601	HEM	CHD-C1D	3.08	1.46	1.39
2	B	601	HEM	CHA-C1A	3.07	1.46	1.39
2	B	601	HEM	C1B-NB	-3.06	1.34	1.40
3	D	602	7AW	C28-N32	3.05	1.37	1.30
2	B	601	HEM	CHD-C1D	3.05	1.46	1.39
2	A	601	HEM	CHB-C4A	3.02	1.46	1.39
2	D	601	HEM	C2A-C3A	3.00	1.46	1.38
2	A	601	HEM	CHB-C1B	2.98	1.44	1.38
2	B	601	HEM	CHB-C1B	2.98	1.44	1.38
2	A	601	HEM	CHC-C4B	2.93	1.45	1.39
2	B	601	HEM	CHB-C4A	2.89	1.45	1.39
2	C	601	HEM	C2A-C3A	2.87	1.46	1.38
2	D	601	HEM	CHB-C1B	2.81	1.44	1.38
2	D	601	HEM	CHA-C1A	2.81	1.45	1.39
2	B	601	HEM	C4D-ND	-2.78	1.35	1.40
3	A	602	7AW	C26-C25	2.73	1.41	1.35
3	A	602	7AW	C28-N32	2.70	1.36	1.30
3	C	602	7AW	C28-N32	2.65	1.36	1.30
2	D	601	HEM	C1B-NB	-2.63	1.35	1.40
3	D	602	7AW	C26-C25	2.63	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C1A-C2A	2.60	1.49	1.44
3	B	602	7AW	C28-N32	2.58	1.36	1.30
3	B	602	7AW	C26-C25	2.55	1.40	1.35
2	B	601	HEM	C4A-C3A	2.52	1.49	1.43
2	A	601	HEM	CHA-C1A	2.51	1.45	1.39
2	C	601	HEM	C4D-C3D	2.50	1.49	1.45
3	C	602	7AW	C26-C25	2.50	1.40	1.35
2	D	601	HEM	CHB-C4A	2.48	1.45	1.39
2	A	601	HEM	C1B-C2B	2.39	1.49	1.44
2	A	601	HEM	C4A-C3A	2.39	1.48	1.43
2	D	601	HEM	C3B-C4B	2.37	1.49	1.44
2	C	601	HEM	C4A-C3A	2.31	1.48	1.43
2	D	601	HEM	C1B-C2B	2.21	1.49	1.44
2	C	601	HEM	C1B-C2B	2.19	1.49	1.44
2	B	601	HEM	C1A-C2A	2.17	1.48	1.44
2	A	601	HEM	C1B-NB	-2.17	1.36	1.40
2	C	601	HEM	C1B-NB	-2.15	1.36	1.40
2	C	601	HEM	O2A-CGA	-2.11	1.23	1.30
2	D	601	HEM	C4A-C3A	2.10	1.48	1.43
2	A	601	HEM	C1D-C2D	2.08	1.48	1.44
2	A	601	HEM	O2A-CGA	-2.03	1.24	1.30

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	C3B-C2B-C1B	-9.48	99.29	106.41
2	A	601	HEM	C3B-C4B-NB	9.44	116.25	109.47
2	D	601	HEM	C3B-C4B-NB	9.14	116.03	109.47
2	B	601	HEM	C3B-C4B-NB	9.10	116.01	109.47
2	D	601	HEM	C2B-C1B-NB	9.09	120.29	109.84
2	C	601	HEM	C3B-C4B-NB	8.80	115.79	109.47
2	D	601	HEM	C3B-C2B-C1B	-8.77	99.83	106.41
2	A	601	HEM	C3B-C2B-C1B	-8.60	99.95	106.41
2	B	601	HEM	C3B-C2B-C1B	-8.25	100.22	106.41
2	B	601	HEM	C2B-C1B-NB	8.23	119.31	109.84
2	A	601	HEM	C2B-C1B-NB	7.73	118.72	109.84
2	C	601	HEM	C2B-C1B-NB	7.50	118.46	109.84
2	C	601	HEM	C2D-C1D-ND	6.61	117.54	109.90
2	B	601	HEM	C2D-C1D-ND	6.60	117.54	109.90
2	D	601	HEM	C2D-C1D-ND	6.43	117.34	109.90
2	B	601	HEM	C3D-C4D-ND	6.12	116.89	110.17
2	A	601	HEM	C3D-C4D-ND	6.10	116.87	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	7AW	C02-C03-C04	-5.97	109.57	114.95
2	D	601	HEM	C1D-C2D-C3D	-5.92	100.75	106.98
2	A	601	HEM	C2D-C1D-ND	5.69	116.48	109.90
2	C	601	HEM	C1D-C2D-C3D	-5.53	101.16	106.98
2	B	601	HEM	C3C-C2C-C1C	-5.41	101.93	107.05
2	C	601	HEM	C2A-C1A-NA	5.27	116.00	110.15
2	B	601	HEM	C1D-C2D-C3D	-5.17	101.54	106.98
2	A	601	HEM	C2A-C1A-NA	5.14	115.86	110.15
2	D	601	HEM	C2A-C1A-NA	4.98	115.68	110.15
2	C	601	HEM	C3D-C4D-ND	4.95	115.60	110.17
2	D	601	HEM	C1B-NB-C4B	-4.91	99.39	105.21
2	D	601	HEM	C4A-NA-C1A	-4.90	97.84	105.82
2	A	601	HEM	C1D-C2D-C3D	-4.89	101.83	106.98
2	C	601	HEM	C3C-C2C-C1C	-4.84	102.47	107.05
2	C	601	HEM	C4A-NA-C1A	-4.83	97.95	105.82
2	D	601	HEM	C3D-C4D-ND	4.79	115.43	110.17
3	A	602	7AW	C04-N36-C37	4.69	129.45	122.23
3	A	602	7AW	S45-C44-N43	-4.66	107.68	115.15
2	A	601	HEM	C3C-C2C-C1C	-4.65	102.64	107.05
3	D	602	7AW	C02-C03-C04	-4.56	110.84	114.95
3	B	602	7AW	S45-C44-N43	-4.49	107.94	115.15
2	D	601	HEM	C3C-C2C-C1C	-4.46	102.82	107.05
3	C	602	7AW	C44-S45-C41	4.45	94.54	89.62
2	B	601	HEM	C4C-NC-C1C	-4.44	98.58	105.82
3	B	602	7AW	O39-C37-N36	4.34	119.73	110.45
3	A	602	7AW	C44-S45-C41	4.31	94.39	89.62
2	D	601	HEM	CBD-CAD-C3D	-4.23	100.83	112.53
3	D	602	7AW	S45-C44-N43	-4.16	108.47	115.15
2	C	601	HEM	CHD-C1D-C2D	-4.16	118.46	125.03
2	A	601	HEM	C4A-NA-C1A	-4.15	99.05	105.82
3	B	602	7AW	O39-C37-O38	-4.10	116.39	124.26
2	D	601	HEM	C3A-C4A-NA	4.10	116.71	110.14
2	A	601	HEM	C1B-NB-C4B	-4.07	100.39	105.21
2	C	601	HEM	CBD-CAD-C3D	-4.04	101.35	112.53
2	B	601	HEM	C2C-C1C-NC	4.01	117.06	109.64
2	B	601	HEM	C1B-NB-C4B	-4.01	100.46	105.21
3	B	602	7AW	C44-S45-C41	4.00	94.04	89.62
3	D	602	7AW	O39-C37-O38	-3.95	116.69	124.26
3	C	602	7AW	C26-S27-C28	3.94	94.19	89.52
3	A	602	7AW	S27-C28-N32	-3.91	109.08	114.19
2	C	601	HEM	CMB-C2B-C1B	3.87	131.09	125.03
3	B	602	7AW	S27-C28-N32	-3.85	109.16	114.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	7AW	C26-S27-C28	3.83	94.06	89.52
3	C	602	7AW	C04-N36-C37	3.83	128.12	122.23
3	C	602	7AW	S45-C44-N43	-3.82	109.02	115.15
3	C	602	7AW	S27-C28-N32	-3.82	109.20	114.19
2	D	601	HEM	C4C-NC-C1C	-3.75	99.71	105.82
2	C	601	HEM	C4C-NC-C1C	-3.73	99.75	105.82
3	C	602	7AW	O39-C37-O38	-3.70	117.16	124.26
2	B	601	HEM	C2A-C1A-NA	3.68	114.24	110.15
2	C	601	HEM	C1B-NB-C4B	-3.66	100.87	105.21
2	B	601	HEM	C4B-C3B-C2B	-3.66	103.91	107.28
3	B	602	7AW	C05-C04-C03	-3.65	106.47	112.41
3	A	602	7AW	C26-S27-C28	3.63	93.82	89.52
3	D	602	7AW	S27-C28-N32	-3.63	109.44	114.19
2	B	601	HEM	C4D-ND-C1D	-3.63	100.91	105.21
3	A	602	7AW	C40-O39-C37	3.62	119.87	115.67
2	A	601	HEM	C4C-NC-C1C	-3.60	99.95	105.82
2	C	601	HEM	C3A-C4A-NA	3.57	115.86	110.14
2	B	601	HEM	C4A-NA-C1A	-3.56	100.01	105.82
2	A	601	HEM	C2C-C1C-NC	3.54	116.19	109.64
2	C	601	HEM	C2C-C1C-NC	3.54	116.18	109.64
3	D	602	7AW	C26-S27-C28	3.52	93.69	89.52
2	B	601	HEM	CBD-CAD-C3D	-3.48	102.90	112.53
3	A	602	7AW	C09-C08-C07	-3.46	106.10	113.71
3	D	602	7AW	C44-S45-C41	3.45	93.44	89.62
2	D	601	HEM	CHD-C1D-C2D	-3.45	119.58	125.03
2	A	601	HEM	CBD-CAD-C3D	-3.42	103.09	112.53
2	D	601	HEM	C2C-C1C-NC	3.41	115.94	109.64
2	B	601	HEM	CHD-C1D-C2D	-3.36	119.72	125.03
3	C	602	7AW	O39-C37-N36	3.25	117.40	110.45
3	C	602	7AW	C02-C03-C04	-3.24	112.03	114.95
2	A	601	HEM	CMB-C2B-C1B	3.22	130.07	125.03
2	A	601	HEM	C3A-C4A-NA	3.19	115.25	110.14
2	C	601	HEM	CHB-C4A-C3A	-3.16	118.25	127.43
2	D	601	HEM	CHB-C1B-C2B	-3.16	117.97	126.95
2	B	601	HEM	C3A-C4A-NA	3.15	115.20	110.14
3	D	602	7AW	C04-N36-C37	3.13	127.05	122.23
2	D	601	HEM	C4B-C3B-C2B	-3.12	104.41	107.28
2	D	601	HEM	CHB-C4A-C3A	-3.10	118.43	127.43
2	B	601	HEM	CHC-C1C-C2C	-3.05	119.15	125.49
3	D	602	7AW	O39-C37-N36	3.02	116.92	110.45
3	A	602	7AW	O39-C37-O38	-3.00	118.52	124.26
3	C	602	7AW	C40-O39-C37	2.97	119.12	115.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	HEM	CMD-C2D-C1D	2.93	129.62	125.03
2	C	601	HEM	CHC-C4B-C3B	-2.93	119.23	125.07
3	B	602	7AW	C02-C03-C04	-2.92	112.31	114.95
2	B	601	HEM	CHB-C1B-C2B	-2.91	118.67	126.95
2	A	601	HEM	C4B-C3B-C2B	-2.91	104.60	107.28
2	A	601	HEM	CMD-C2D-C1D	2.90	129.56	125.03
3	C	602	7AW	C05-C04-C03	-2.89	107.70	112.41
2	A	601	HEM	C4D-C3D-C2D	-2.89	102.69	106.89
2	A	601	HEM	CHD-C1D-C2D	-2.87	120.50	125.03
3	D	602	7AW	C42-N43-C44	2.87	115.30	110.24
3	B	602	7AW	C42-N43-C44	2.82	115.23	110.24
2	C	601	HEM	CHB-C1B-NB	-2.82	120.87	124.37
2	C	601	HEM	C4D-ND-C1D	-2.81	101.88	105.21
2	B	601	HEM	CAD-C3D-C4D	2.78	129.54	124.70
3	A	602	7AW	O39-C37-N36	2.78	116.39	110.45
2	A	601	HEM	CHA-C1A-C2A	-2.76	119.25	125.30
2	A	601	HEM	CHC-C4B-C3B	-2.74	119.61	125.07
3	A	602	7AW	C42-N43-C44	2.72	115.05	110.24
2	B	601	HEM	CHB-C4A-C3A	-2.70	119.60	127.43
2	A	601	HEM	C4D-ND-C1D	-2.69	102.02	105.21
2	B	601	HEM	C4D-C3D-C2D	-2.68	103.00	106.89
2	D	601	HEM	C4D-ND-C1D	-2.63	102.09	105.21
2	D	601	HEM	CAA-CBA-CGA	-2.62	106.72	113.67
2	B	601	HEM	CMD-C2D-C1D	2.62	129.12	125.03
2	D	601	HEM	CMB-C2B-C1B	2.60	129.10	125.03
2	D	601	HEM	CHC-C1C-C2C	-2.59	120.11	125.49
3	D	602	7AW	C03-C04-N36	2.58	114.74	110.50
3	C	602	7AW	C25-C26-S27	-2.58	107.15	110.59
3	A	602	7AW	C05-C04-C03	-2.56	108.24	112.41
2	A	601	HEM	CHB-C1B-NB	-2.54	121.22	124.37
2	B	601	HEM	CHD-C4C-C3C	-2.54	120.93	125.21
3	B	602	7AW	C25-C26-S27	-2.52	107.23	110.59
2	C	601	HEM	CMC-C2C-C1C	2.51	129.15	124.73
2	A	601	HEM	CHB-C4A-C3A	-2.50	120.16	127.43
3	D	602	7AW	C40-O39-C37	2.50	118.57	115.67
2	D	601	HEM	CHA-C1A-C2A	-2.48	119.88	125.30
2	A	601	HEM	CHB-C1B-C2B	-2.47	119.92	126.95
2	A	601	HEM	CHA-C4D-C3D	-2.47	120.67	125.23
2	C	601	HEM	CHA-C1A-C2A	-2.46	119.92	125.30
2	C	601	HEM	CHC-C1C-C2C	-2.45	120.40	125.49
2	A	601	HEM	CHC-C1C-C2C	-2.42	120.44	125.49
3	A	602	7AW	C03-C04-N36	2.41	114.45	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	7AW	C09-C08-C07	-2.39	108.44	113.71
2	B	601	HEM	CMA-C3A-C4A	2.36	129.01	125.42
2	C	601	HEM	CMD-C2D-C1D	2.34	128.69	125.03
2	B	601	HEM	C4A-C3A-C2A	-2.31	104.17	106.82
3	C	602	7AW	C05-C04-N36	2.31	114.28	110.50
2	C	601	HEM	CAA-C2A-C1A	2.30	129.44	124.94
3	A	602	7AW	C25-C26-S27	-2.30	107.52	110.59
3	C	602	7AW	C06-C07-N15	2.29	114.25	110.50
2	B	601	HEM	CHA-C1A-C2A	-2.28	120.30	125.30
2	C	601	HEM	CAD-C3D-C4D	2.28	128.67	124.70
2	C	601	HEM	CHB-C1B-C2B	-2.24	120.58	126.95
2	D	601	HEM	C4A-C3A-C2A	-2.22	104.27	106.82
2	D	601	HEM	C1C-CHC-C4B	-2.21	121.32	126.02
3	D	602	7AW	C09-C08-C07	-2.21	108.85	113.71
3	D	602	7AW	C33-C18-C16	-2.21	106.00	111.38
2	B	601	HEM	CHA-C4D-C3D	-2.21	121.16	125.23
2	A	601	HEM	CMC-C2C-C1C	2.20	128.61	124.73
2	C	601	HEM	C4D-C3D-C2D	-2.16	103.74	106.89
2	B	601	HEM	CHA-C4D-ND	-2.15	121.71	124.37
2	D	601	HEM	CHB-C1B-NB	-2.14	121.72	124.37
2	D	601	HEM	CHD-C4C-C3C	-2.14	121.61	125.21
2	B	601	HEM	CHC-C4B-C3B	-2.13	120.81	125.07
2	C	601	HEM	C4A-CHB-C1B	-2.10	121.31	126.25
2	B	601	HEM	CMC-C2C-C1C	2.09	128.41	124.73
2	D	601	HEM	C1A-CHA-C4D	-2.09	121.34	126.25
2	B	601	HEM	CHB-C1B-NB	-2.08	121.79	124.37
2	D	601	HEM	CHA-C4D-C3D	-2.07	121.40	125.23
2	D	601	HEM	CHC-C4B-C3B	-2.07	120.94	125.07
2	D	601	HEM	CAA-C2A-C1A	2.06	128.96	124.94
2	D	601	HEM	CMA-C3A-C4A	2.04	128.53	125.42
2	B	601	HEM	C1C-CHC-C4B	-2.04	121.69	126.02
2	C	601	HEM	CHA-C4D-ND	-2.00	121.89	124.37

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	HEM	C2C-C3C-CAC-CBC
2	C	601	HEM	C2B-C3B-CAB-CBB
2	D	601	HEM	C2B-C3B-CAB-CBB
3	A	602	7AW	C03-C04-N36-C37
3	A	602	7AW	C02-C03-C04-C05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	602	7AW	N36-C04-C05-C06
3	A	602	7AW	C03-C04-C05-C06
3	A	602	7AW	C06-C07-C08-C09
3	A	602	7AW	N15-C07-C08-C09
3	A	602	7AW	O21-C20-N19-C18
3	A	602	7AW	N22-C20-N19-C18
3	A	602	7AW	N19-C20-N22-C23
3	A	602	7AW	N19-C20-N22-C24
3	A	602	7AW	O21-C20-N22-C23
3	A	602	7AW	O21-C20-N22-C24
3	B	602	7AW	C03-C04-N36-C37
3	B	602	7AW	C02-C03-C04-C05
3	B	602	7AW	C04-C05-C06-C07
3	B	602	7AW	C06-C07-C08-C09
3	B	602	7AW	N15-C07-C08-C09
3	B	602	7AW	O21-C20-N19-C18
3	B	602	7AW	N22-C20-N19-C18
3	B	602	7AW	N19-C20-N22-C23
3	B	602	7AW	N19-C20-N22-C24
3	B	602	7AW	O21-C20-N22-C23
3	B	602	7AW	O21-C20-N22-C24
3	C	602	7AW	C03-C04-N36-C37
3	C	602	7AW	C03-C04-C05-C06
3	C	602	7AW	C06-C07-C08-C09
3	C	602	7AW	N15-C07-C08-C09
3	C	602	7AW	C16-C18-C33-C35
3	C	602	7AW	C16-C18-C33-C34
3	C	602	7AW	O21-C20-N19-C18
3	C	602	7AW	N22-C20-N19-C18
3	C	602	7AW	N19-C20-N22-C23
3	C	602	7AW	N19-C20-N22-C24
3	C	602	7AW	O21-C20-N22-C23
3	C	602	7AW	O21-C20-N22-C24
3	D	602	7AW	C03-C04-N36-C37
3	D	602	7AW	C03-C04-C05-C06
3	D	602	7AW	C06-C07-C08-C09
3	D	602	7AW	N15-C07-C08-C09
3	D	602	7AW	O21-C20-N19-C18
3	D	602	7AW	N22-C20-N19-C18
3	D	602	7AW	N19-C20-N22-C23
3	D	602	7AW	N19-C20-N22-C24
3	D	602	7AW	O21-C20-N22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	602	7AW	O21-C20-N22-C24
3	C	602	7AW	O17-C16-N15-C07
3	D	602	7AW	O17-C16-N15-C07
3	D	602	7AW	C18-C16-N15-C07
3	D	602	7AW	N19-C18-C33-C35
3	C	602	7AW	C18-C16-N15-C07
3	D	602	7AW	O38-C37-O39-C40
3	D	602	7AW	C16-C18-C33-C35
3	C	602	7AW	N19-C18-C33-C35
3	D	602	7AW	N19-C18-C33-C34
3	B	602	7AW	O39-C37-N36-C04
3	C	602	7AW	N19-C18-C33-C34
3	B	602	7AW	O38-C37-N36-C04
3	D	602	7AW	C16-C18-C33-C34
3	D	602	7AW	N36-C37-O39-C40
3	A	602	7AW	N19-C18-C33-C34
3	B	602	7AW	C18-C16-N15-C07
3	B	602	7AW	O17-C16-N15-C07
3	C	602	7AW	N36-C04-C05-C06
3	D	602	7AW	N36-C04-C05-C06
3	A	602	7AW	C16-C18-C33-C34
3	A	602	7AW	C16-C18-C33-C35
3	A	602	7AW	N19-C18-C33-C35
3	A	602	7AW	O39-C37-N36-C04
3	A	602	7AW	O38-C37-N36-C04
3	C	602	7AW	O38-C37-O39-C40
3	C	602	7AW	N36-C37-O39-C40
2	C	601	HEM	C2C-C3C-CAC-CBC
2	B	601	HEM	C4C-C3C-CAC-CBC
2	C	601	HEM	C4B-C3B-CAB-CBB
2	D	601	HEM	C4B-C3B-CAB-CBB
3	A	602	7AW	N32-C28-C29-C30
3	D	602	7AW	N32-C28-C29-C31
3	B	602	7AW	C01-C02-C03-C04
3	A	602	7AW	C01-C02-C03-C04
3	C	602	7AW	C01-C02-C03-C04
2	A	601	HEM	C2C-C3C-CAC-CBC
2	D	601	HEM	C2C-C3C-CAC-CBC
3	B	602	7AW	C02-C03-C04-N36
3	C	602	7AW	C02-C03-C04-C05
3	D	602	7AW	C02-C03-C04-C05
3	C	602	7AW	C04-C05-C06-C07

Continued on next page...

Continued from previous page...

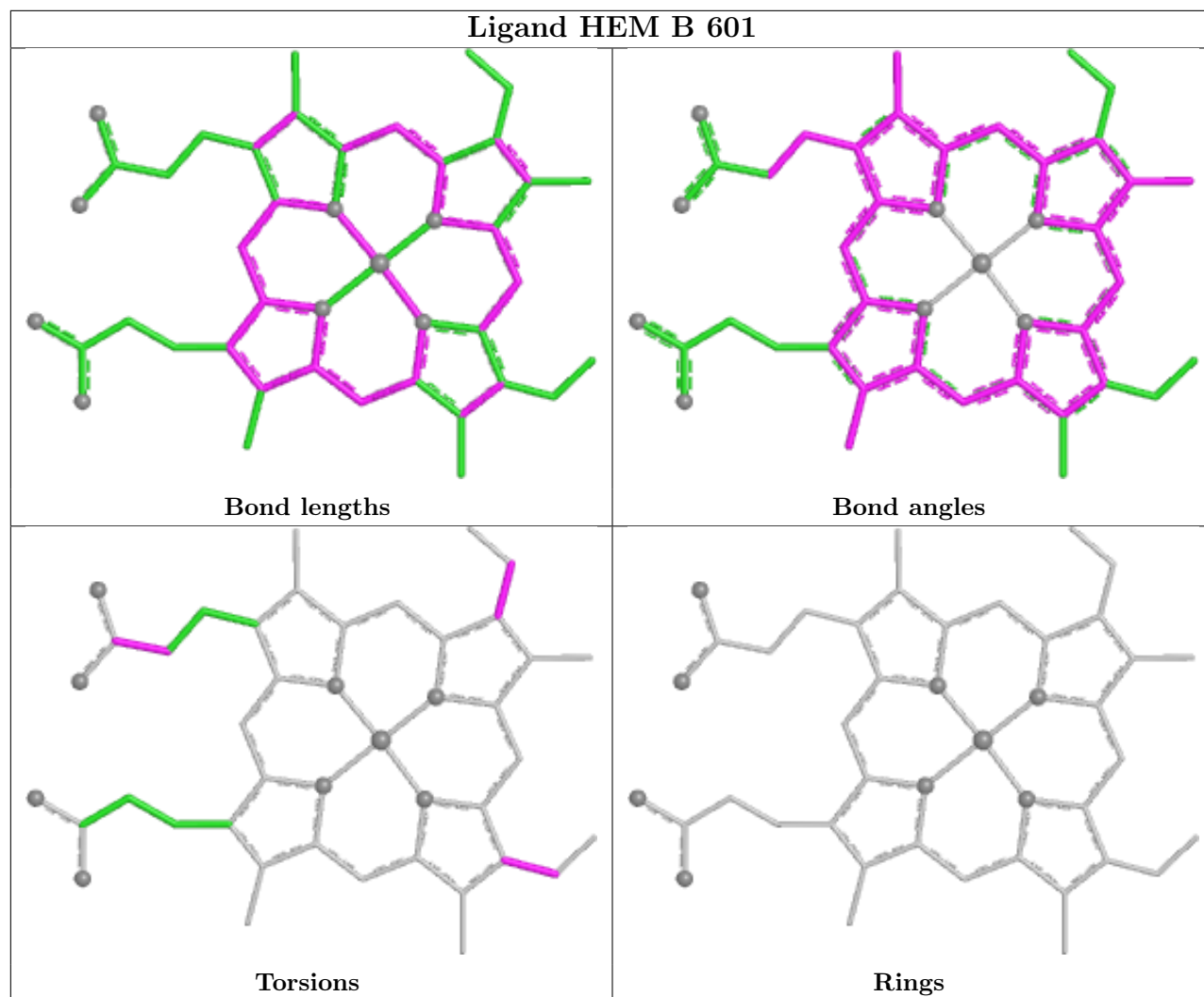
Mol	Chain	Res	Type	Atoms
3	C	602	7AW	N32-C28-C29-C31
3	B	602	7AW	C05-C04-N36-C37
2	C	601	HEM	C4C-C3C-CAC-CBC
2	D	601	HEM	C4C-C3C-CAC-CBC
3	A	602	7AW	C33-C18-N19-C20
3	B	602	7AW	N32-C28-C29-C31
3	D	602	7AW	N32-C28-C29-C30
2	A	601	HEM	C4C-C3C-CAC-CBC
2	B	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	C2B-C3B-CAB-CBB
3	A	602	7AW	C02-C03-C04-N36

There are no ring outliers.

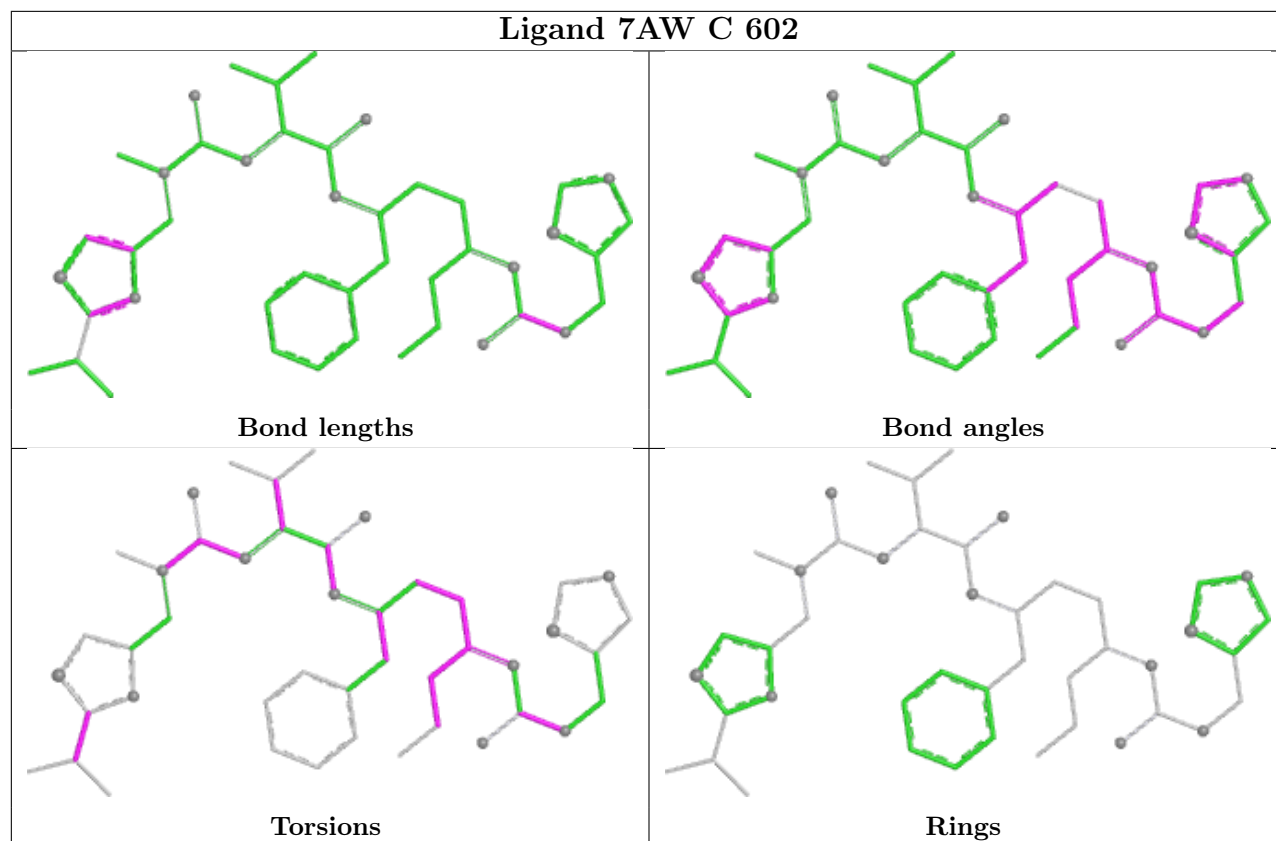
8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	6	0
3	C	602	7AW	4	0
3	A	602	7AW	8	0
3	B	602	7AW	5	0
3	D	602	7AW	4	0
2	D	601	HEM	11	0
2	C	601	HEM	8	0
2	A	601	HEM	8	0

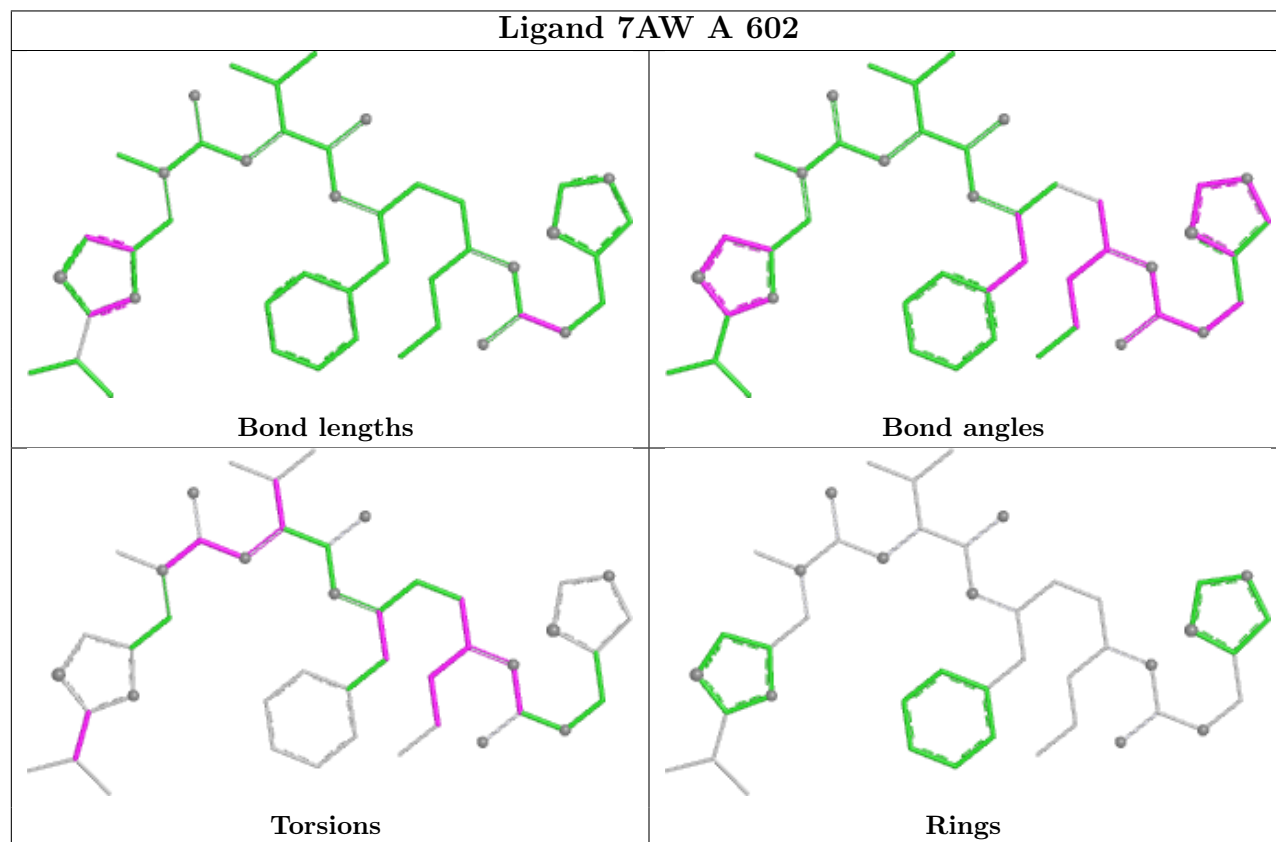
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



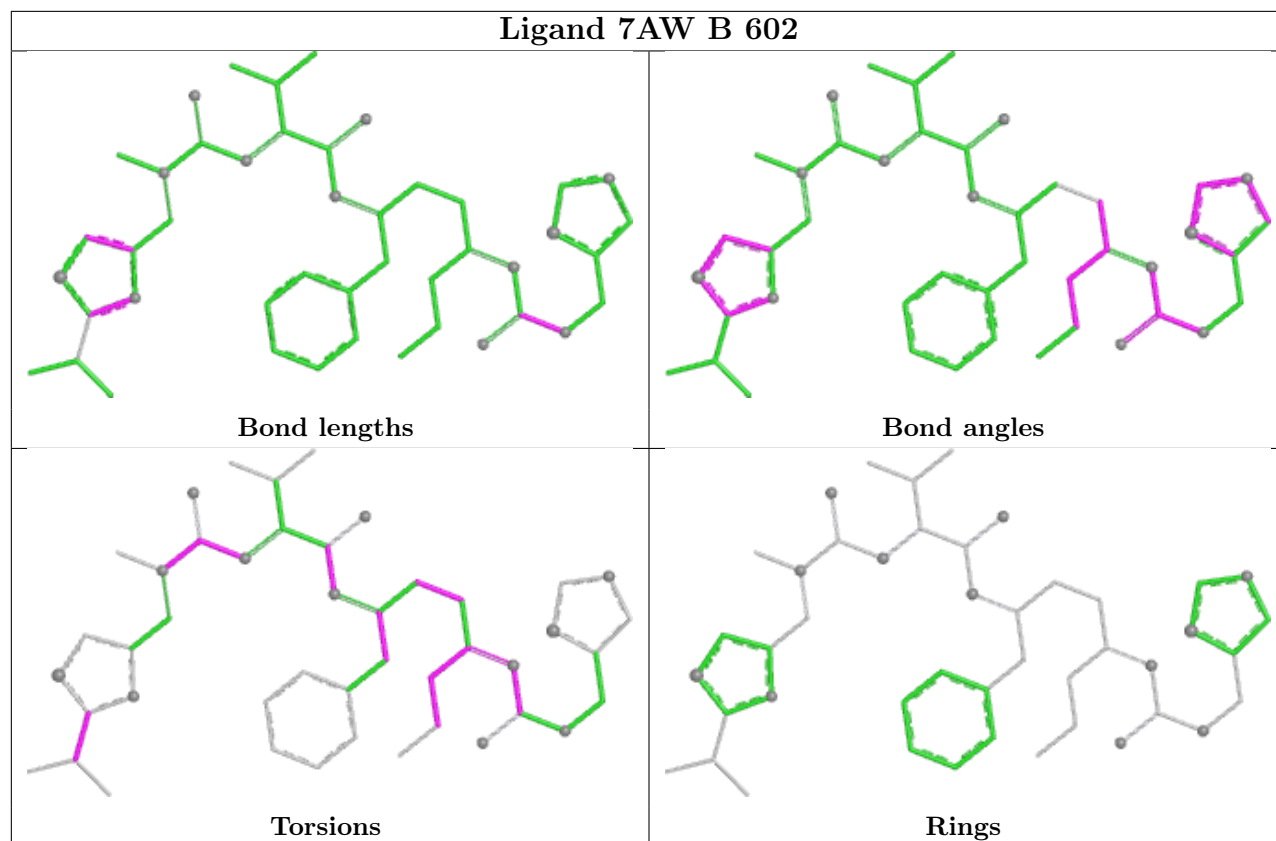
Ligand 7AW C 602



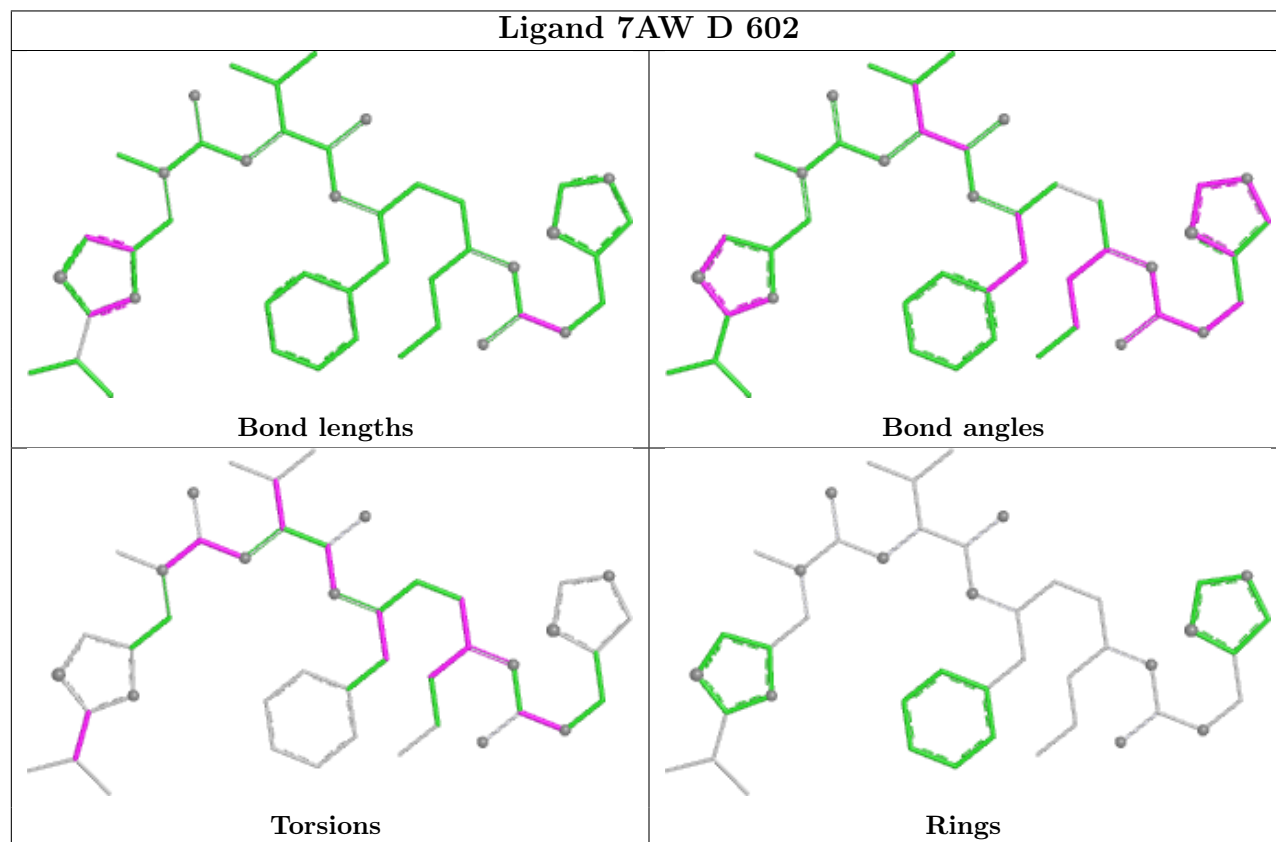
Ligand 7AW A 602

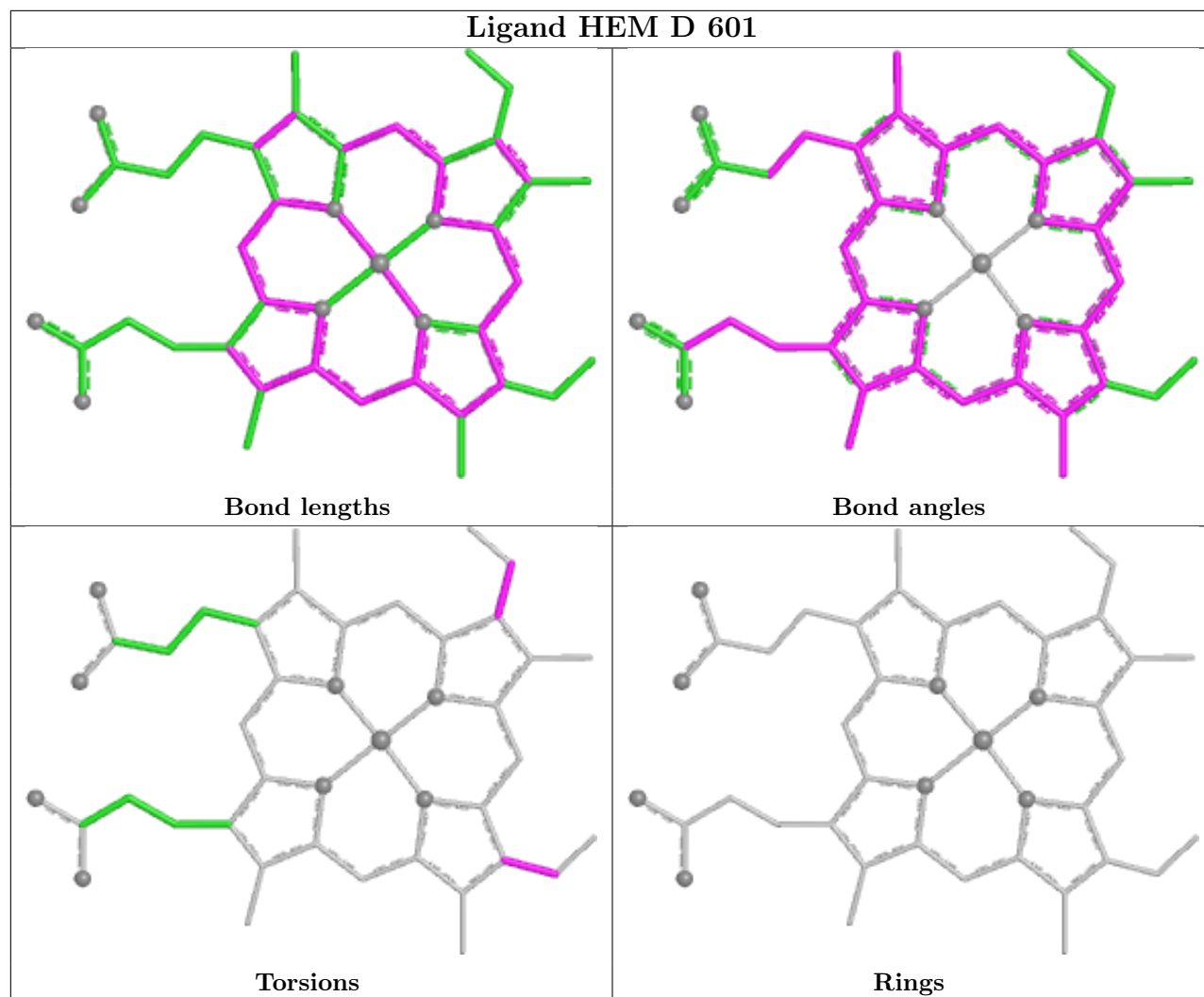


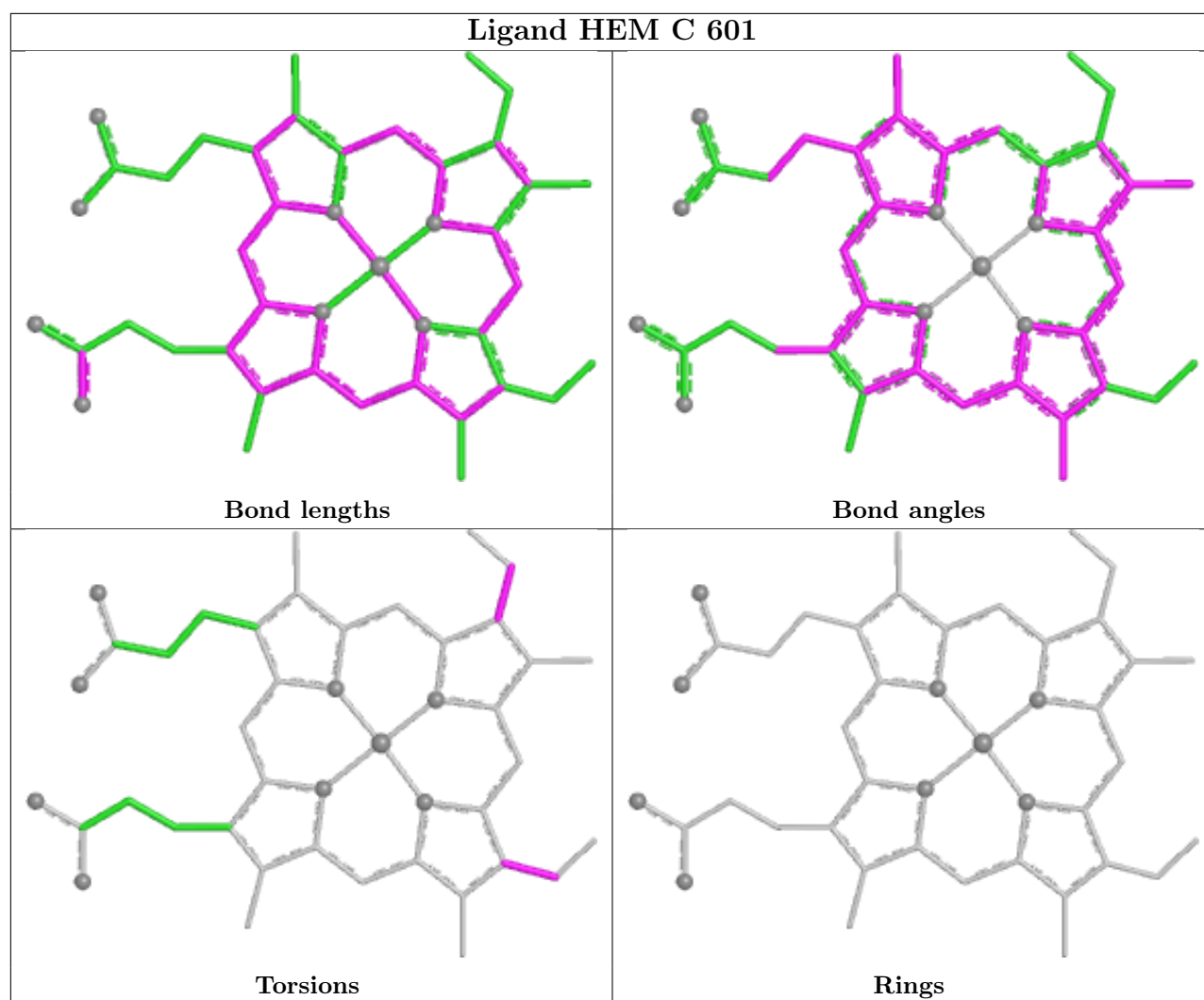
Ligand 7AW B 602

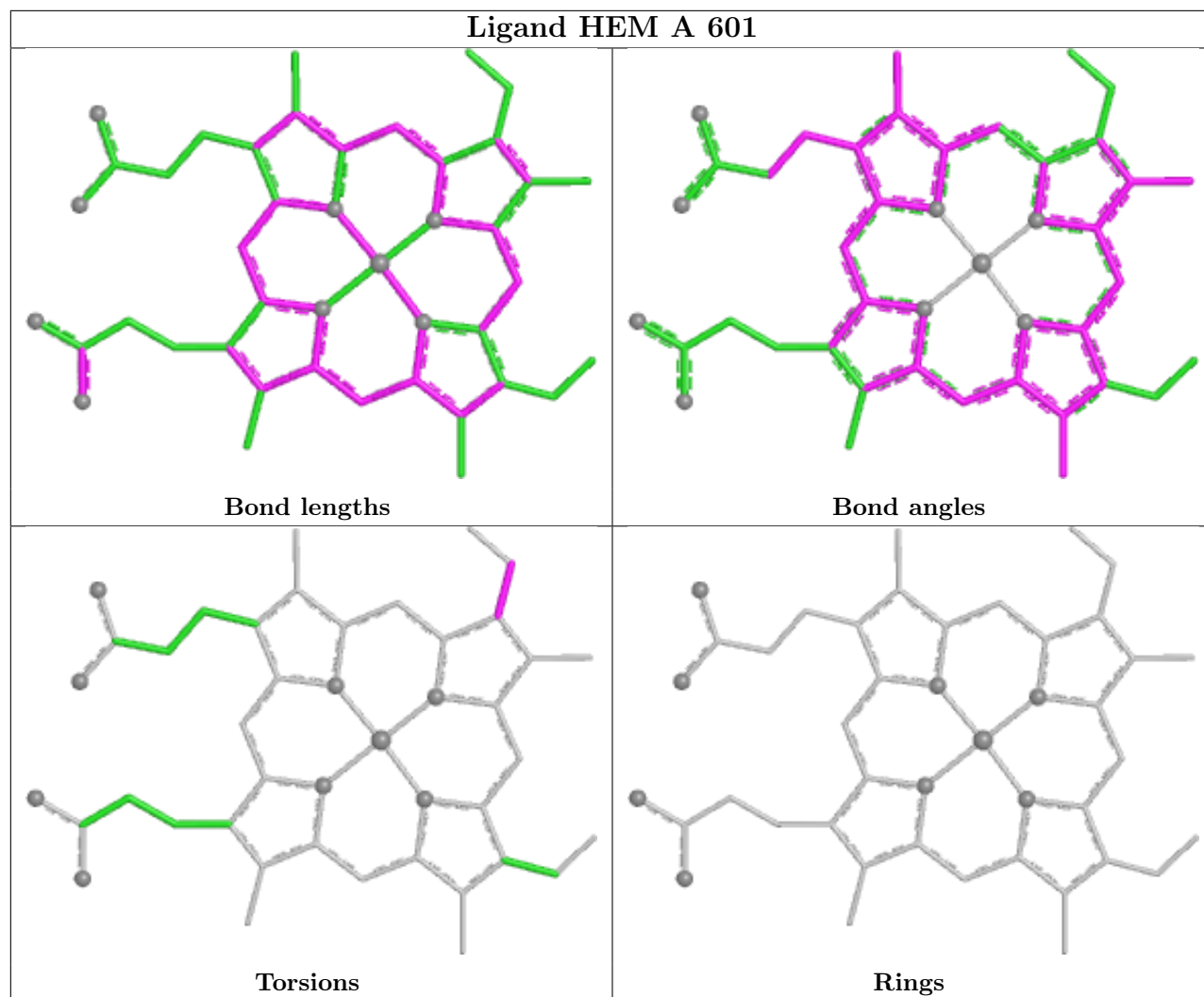


Ligand 7AW D 602









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	458/487 (94%)	0.08	1 (0%) 91 89	35, 57, 80, 103	0
1	B	457/487 (93%)	0.03	2 (0%) 88 86	35, 58, 80, 110	1 (0%)
1	C	458/487 (94%)	0.12	4 (0%) 81 78	36, 59, 85, 104	0
1	D	458/487 (94%)	0.25	9 (1%) 65 60	38, 61, 87, 113	0
All	All	1831/1948 (93%)	0.12	16 (0%) 81 78	35, 59, 84, 113	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	PHE	3.7
1	D	264	THR	3.3
1	D	225	VAL	2.9
1	B	225	VAL	2.7
1	D	226	PHE	2.7
1	C	482	LEU	2.6
1	D	337	ALA	2.6
1	C	215	PHE	2.5
1	A	228	PHE	2.4
1	D	473	ILE	2.4
1	D	108	PHE	2.4
1	D	481	GLY	2.3
1	B	226	PHE	2.3
1	C	289	ALA	2.1
1	D	340	PRO	2.1
1	D	289	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

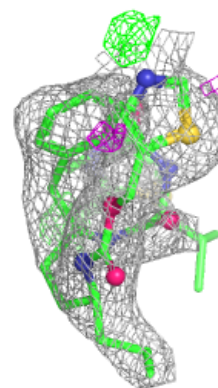
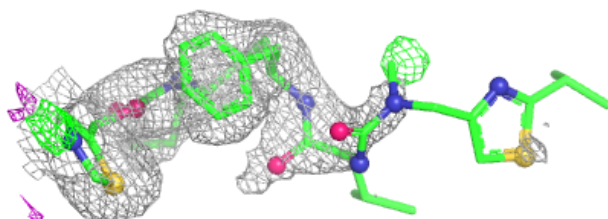
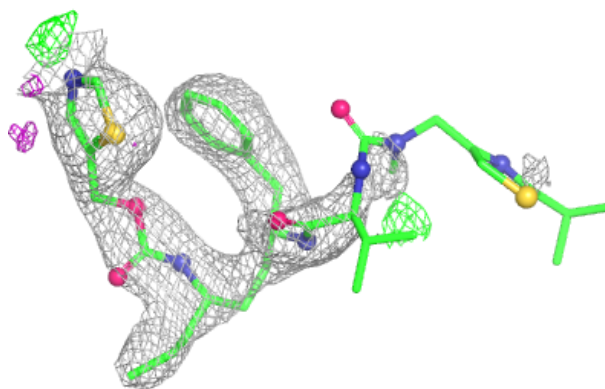
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	7AW	B	602	45/45	0.88	0.16	55,72,154,157	0
3	7AW	D	602	45/45	0.89	0.15	53,78,106,110	0
3	7AW	C	602	45/45	0.90	0.14	42,68,120,121	0
3	7AW	A	602	45/45	0.90	0.14	51,68,94,95	0
2	HEM	A	601	43/43	0.98	0.07	31,35,39,40	0
2	HEM	B	601	43/43	0.98	0.08	36,45,49,50	0
2	HEM	C	601	43/43	0.98	0.08	38,40,43,44	0
2	HEM	D	601	43/43	0.98	0.07	42,44,46,47	0

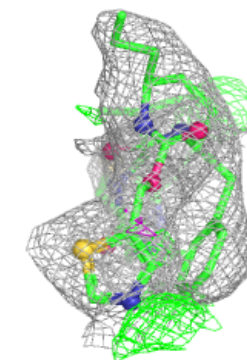
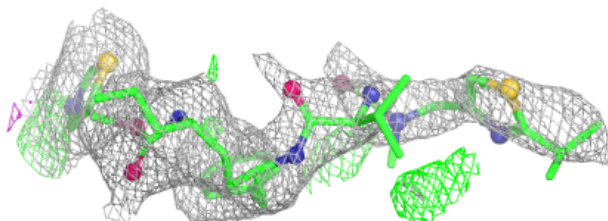
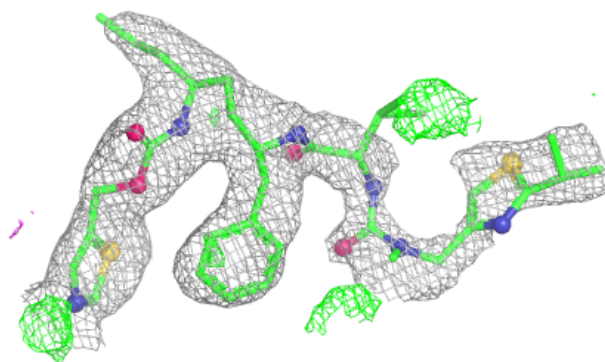
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7AW B 602:

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

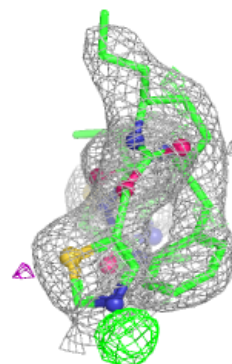
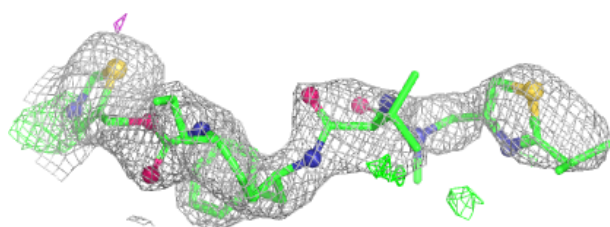
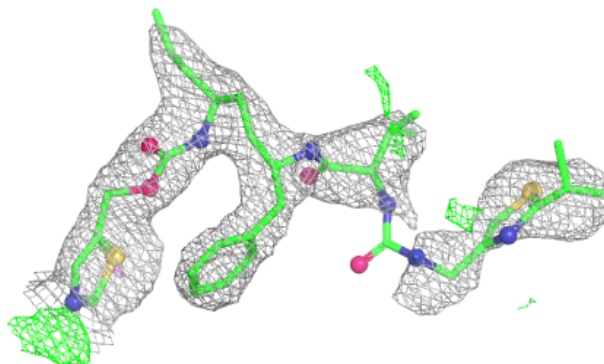
**Electron density around 7AW D 602:**

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

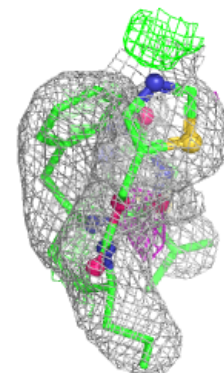
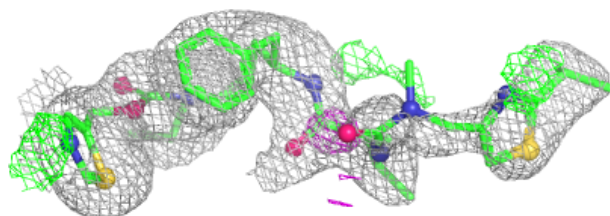
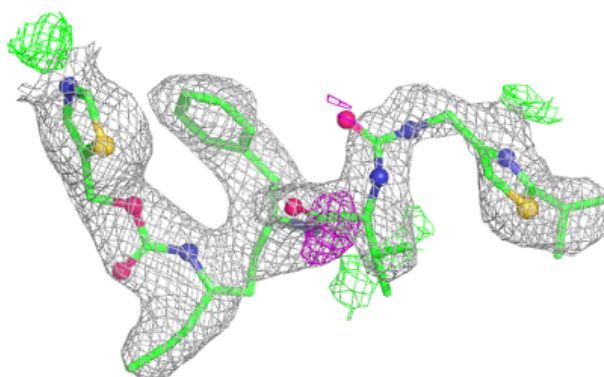


Electron density around 7AW C 602:

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

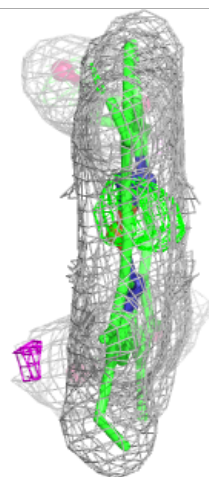
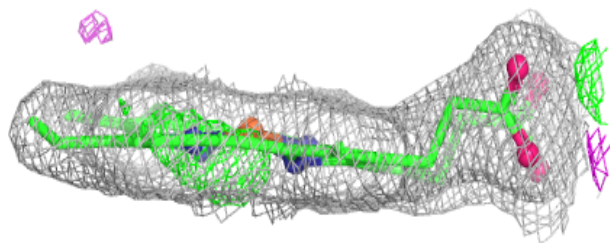
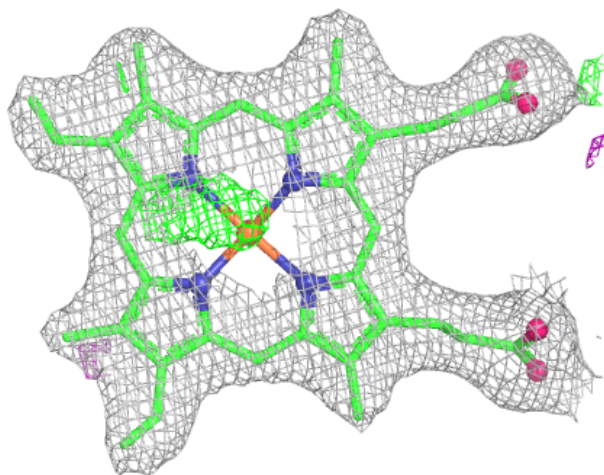
**Electron density around 7AW A 602:**

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



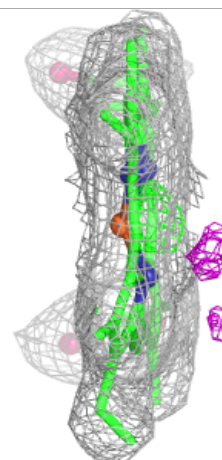
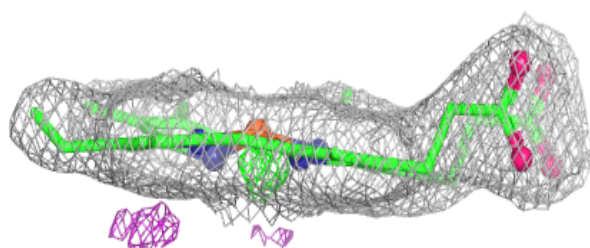
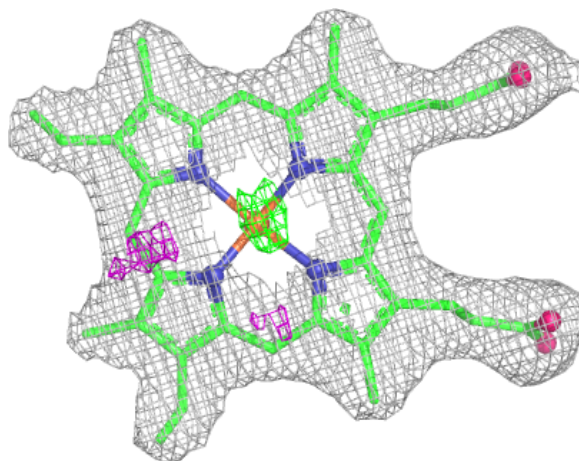
Electron density around HEM A 601:

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



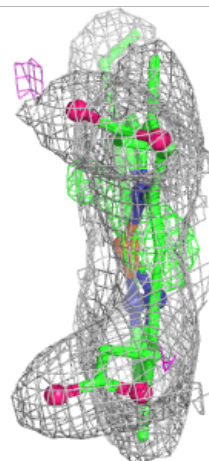
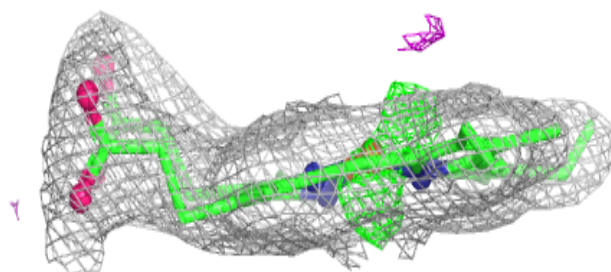
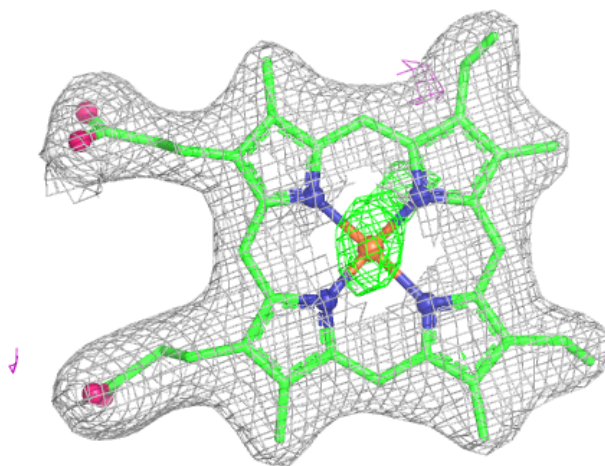
Electron density around HEM B 601:

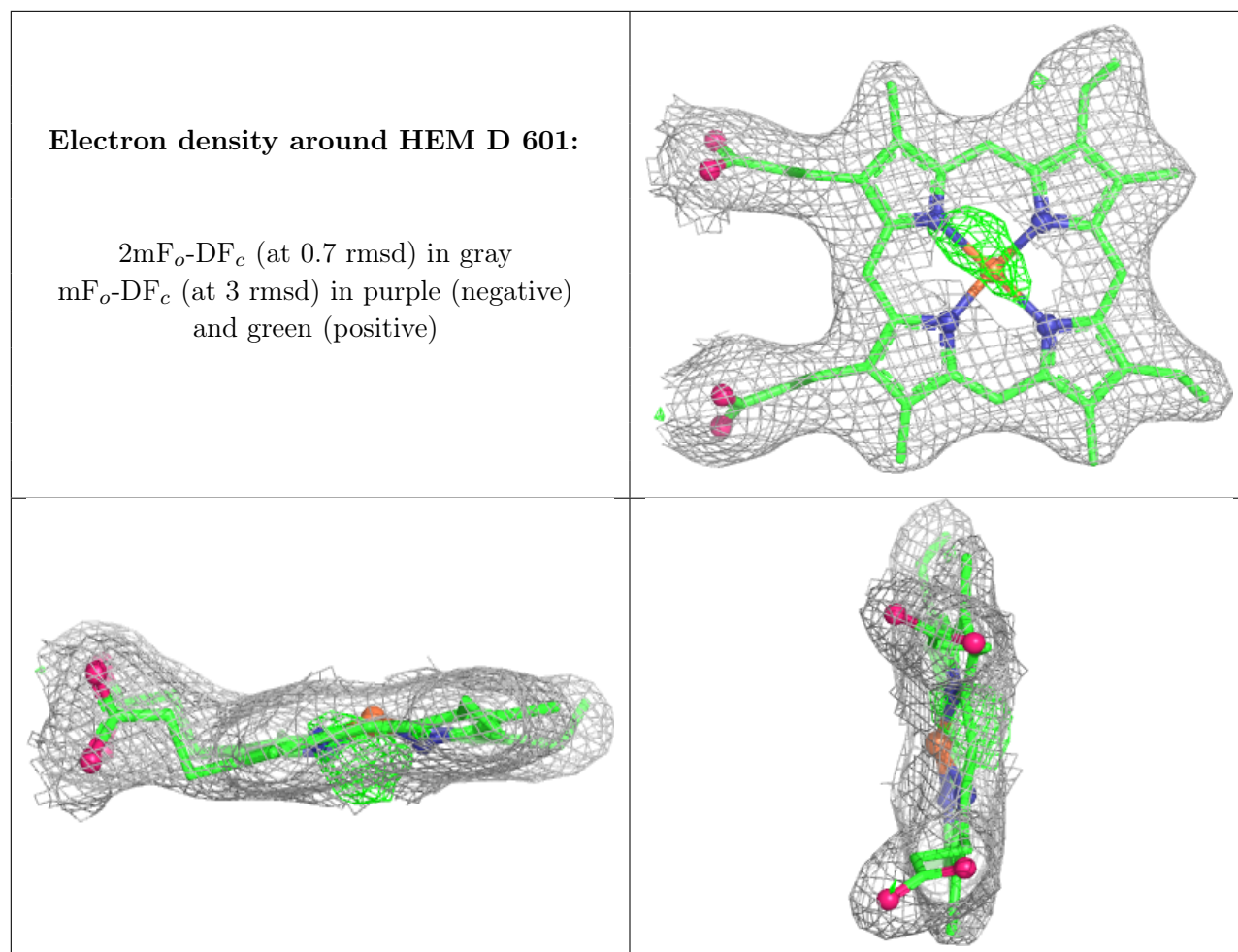
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.