



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:16 AM UTC

PDB ID : 8HID / pdb_00008hid
Title : HUMAN ERYTHROCYTE CATALASE COMPLEXED WITH BT-Br
Authors : Lin, H.-Y.; Yang, G.-F.
Deposited on : 2022-11-19
Resolution : 2.20 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

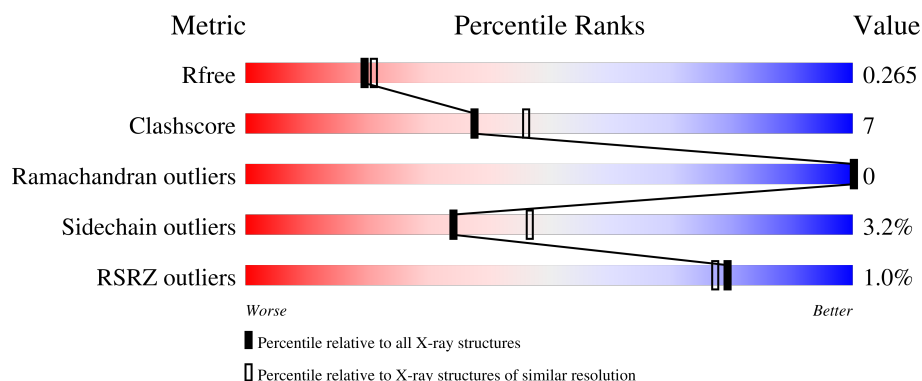
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	527	74% 19% • 6%
1	B	527	76% 17% • 6%
1	C	527	79% 15% • 5%
1	D	527	76% 18% • 6%

2 Entry composition [i](#)

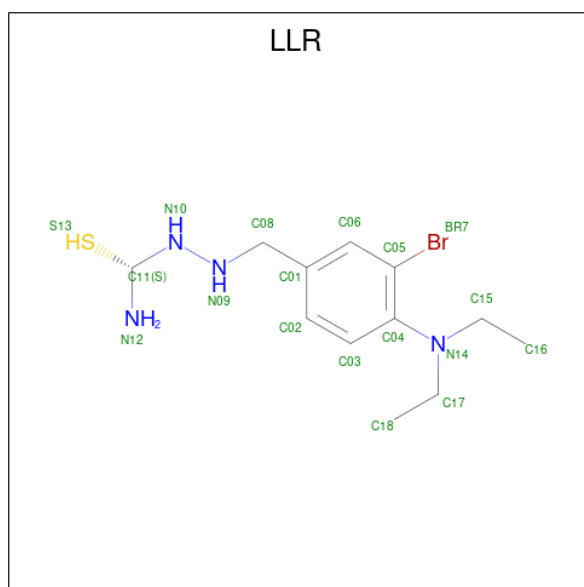
There are 4 unique types of molecules in this entry. The entry contains 18034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4000	2543	708	736	13			
1	B	498	Total	C	N	O	S	0	0	0
			3992	2538	706	735	13			
1	C	499	Total	C	N	O	S	0	0	0
			4006	2546	709	738	13			
1	D	498	Total	C	N	O	S	0	0	0
			3996	2540	707	736	13			

- Molecule 2 is ({S})-azanyl-[2-[[3-bromanyl-4-(diethylamino)phenyl]methyl]hydrazinyl]methanethiol (CCD ID: LLR) (formula: C₁₂H₂₁BrN₄S).



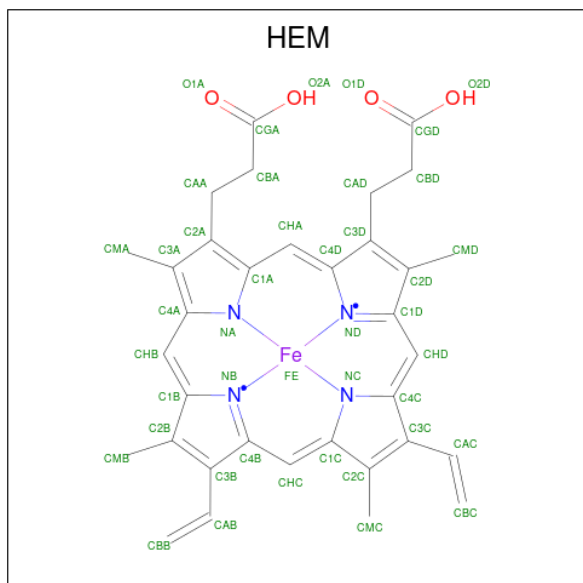
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	S	0
			18	1	12	4	1	0
2	B	1	Total	Br	C	N	S	0
			18	1	12	4	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 18	Br 1	C 12	N 4	S 1	0	0
2	D	1	Total 18	Br 1	C 12	N 4	S 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	491	Total O 491 491	0	0
4	B	475	Total O 475 475	0	0
4	C	440	Total O 440 440	0	0

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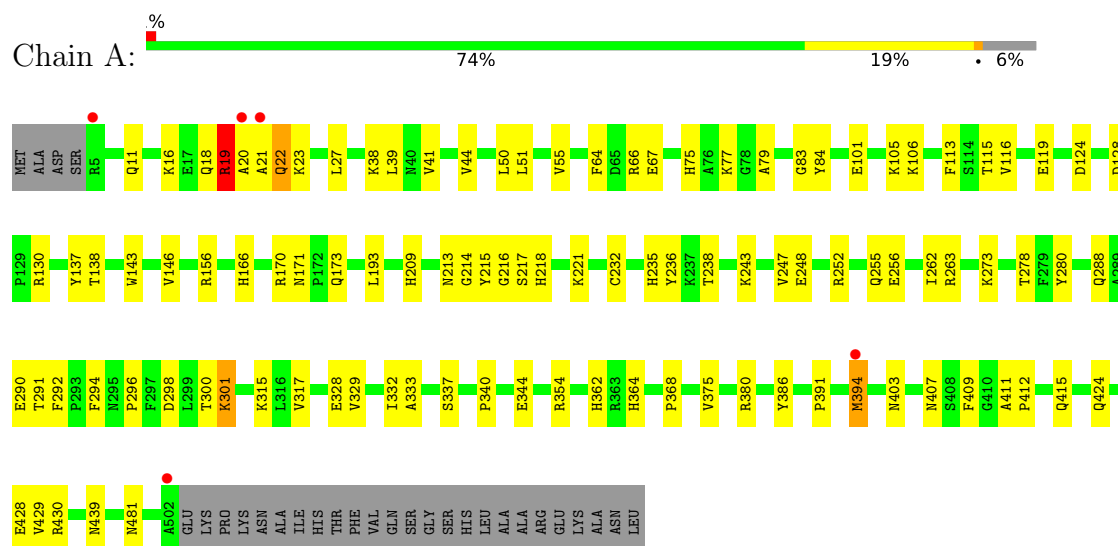
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	390	Total 390	O 390	0	0

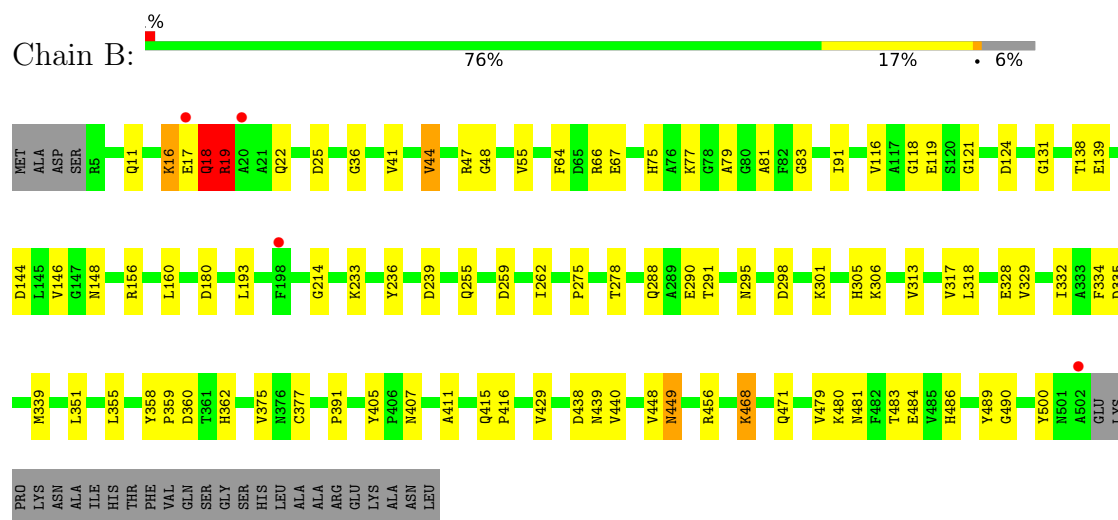
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

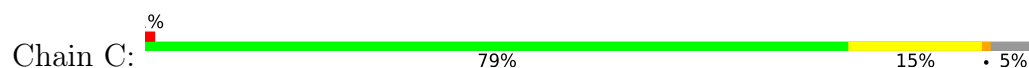
• Molecule 1: Catalase

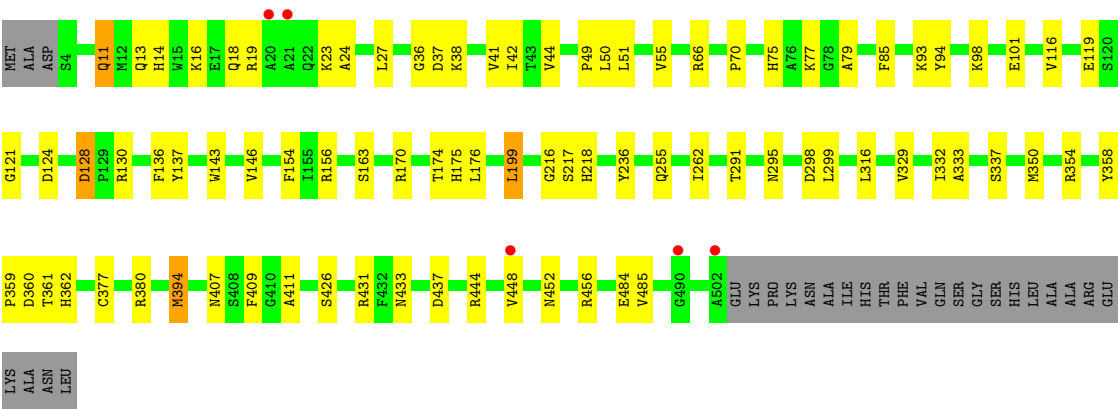


• Molecule 1: Catalase

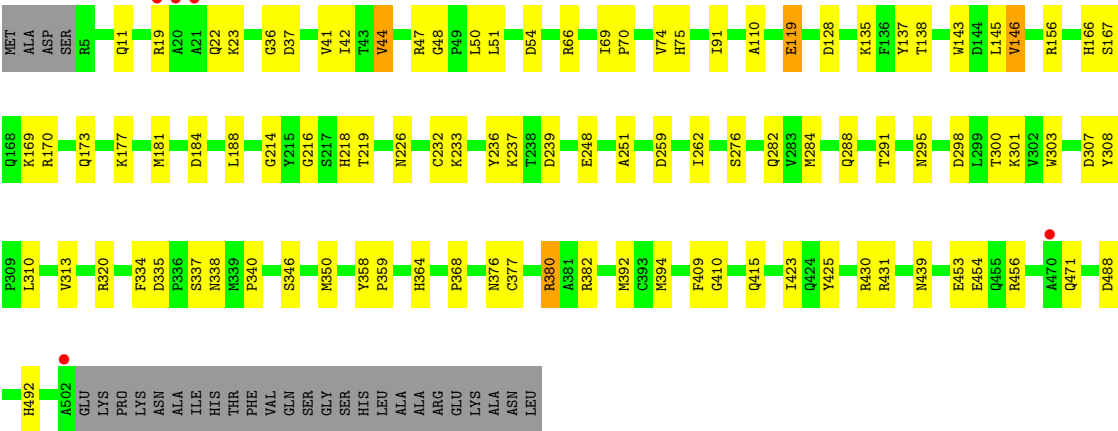


• Molecule 1: Catalase





• Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.47Å 140.87Å 233.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 2.20 39.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.57-2.20) 99.3 (39.57-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.225 , 0.265 0.226 , 0.265	Depositor DCC
R_{free} test set	6972 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18034	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	1/4119 (0.0%)	0.43	2/5598 (0.0%)
1	B	0.27	2/4111 (0.0%)	0.45	6/5589 (0.1%)
1	C	0.28	1/4125 (0.0%)	0.39	0/5606
1	D	0.14	0/4115	0.35	0/5594
All	All	0.27	4/16470 (0.0%)	0.40	8/22387 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	GLN	C-O	-5.80	1.18	1.24
1	A	217	SER	C-O	-5.64	1.16	1.24
1	B	17	GLU	C-O	5.32	1.30	1.24
1	C	24	ALA	C-O	-5.10	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	GLU	CB-CA-C	8.84	125.46	110.79
1	A	22	GLN	N-CA-C	-6.74	97.98	109.24
1	B	18	GLN	N-CA-C	6.07	117.90	111.28
1	B	22	GLN	N-CA-C	5.71	117.33	109.29
1	B	17	GLU	CB-CG-CD	5.57	122.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	N-CA-C	5.17	117.82	111.82
1	A	19	ARG	N-CA-C	-5.08	105.66	111.14
1	B	22	GLN	CB-CA-C	-5.03	108.11	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ARG	Peptide

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	4000	0	3827	69	0
1	B	3992	0	3810	65	0
1	C	4006	0	3832	55	0
1	D	3996	0	3816	68	0
2	A	18	0	0	1	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
2	D	18	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	3	0
3	C	43	0	30	2	0
3	D	43	0	30	3	0
4	A	491	0	0	9	0
4	B	475	0	0	8	0
4	C	440	0	0	1	0
4	D	390	0	0	9	0
All	All	18034	0	15405	222	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 7.

All (222) 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:394:MET:HG2	1:C:394:MET:HG2	1.62	0.81
1:C:79:ALA:HB2	1:C:262:ILE:HG12	1.68	0.76
1:A:409:PHE:HA	1:C:16:LYS:HD3	1.67	0.75
1:A:328:GLU:HA	1:A:375:VAL:HG11	1.68	0.74
1:D:156:ARG:NH2	1:D:439:ASN:OD1	2.23	0.72
1:B:339:MET:SD	4:B:998:HOH:O	2.46	0.71
1:A:79:ALA:HB2	1:A:262:ILE:HG12	1.75	0.69
1:A:298:ASP:HB3	1:A:301:LYS:HG3	1.75	0.67
1:B:328:GLU:HA	1:B:375:VAL:HG11	1.76	0.67
1:B:19:ARG:HG2	1:D:410:GLY:O	1.95	0.66
1:A:407:ASN:HD21	1:A:411:ALA:HB3	1.59	0.66
1:D:75:HIS:NE2	4:D:712:HOH:O	2.29	0.66
1:B:193:LEU:HD21	1:B:481:ASN:HB3	1.78	0.65
1:A:105:LYS:NZ	4:A:709:HOH:O	2.29	0.64
1:A:156:ARG:NH2	1:A:439:ASN:OD1	2.30	0.64
1:B:18:GLN:HB3	4:B:1053:HOH:O	1.97	0.63
1:A:252:ARG:NH1	1:A:256:GLU:OE2	2.32	0.63
1:C:77:LYS:NZ	1:C:124:ASP:OD1	2.31	0.62
1:A:170:ARG:NH1	1:B:259:ASP:OD2	2.32	0.62
1:B:79:ALA:HB2	1:B:262:ILE:HG12	1.82	0.61
3:C:602:HEM:HMB2	3:C:602:HEM:HBB2	1.83	0.61
3:D:602:HEM:HMC1	3:D:602:HEM:HBC2	1.81	0.61
1:D:320:ARG:NH1	4:D:720:HOH:O	2.33	0.60
1:B:146:VAL:HG22	1:B:334:PHE:HB3	1.83	0.60
1:B:77:LYS:NZ	1:B:124:ASP:OD1	2.34	0.59
3:B:602:HEM:HMC1	3:B:602:HEM:HBC2	1.84	0.59
1:D:156:ARG:NH1	1:D:300:THR:OG1	2.35	0.59
1:A:143:TRP:HB2	1:A:340:PRO:HD3	1.84	0.59
1:A:51:LEU:HD13	1:B:429:VAL:HG13	1.84	0.59
1:C:444:ARG:NE	1:C:485:VAL:O	2.33	0.59
1:B:480:LYS:NZ	4:B:726:HOH:O	2.35	0.59
3:D:602:HEM:HMB1	3:D:602:HEM:HBB2	1.83	0.58
1:A:243:LYS:NZ	4:A:718:HOH:O	2.36	0.58
3:A:602:HEM:HMC1	3:A:602:HEM:HBC2	1.86	0.58
1:B:11:GLN:NE2	4:B:728:HOH:O	2.36	0.57
1:D:42:ILE:HG22	1:D:51:LEU:HD12	1.86	0.57
1:A:278:THR:OG1	1:A:315:LYS:NZ	2.35	0.57
1:D:19:ARG:NH2	1:D:23:LYS:O	2.27	0.56
1:D:219:THR:O	1:D:346:SER:OG	2.22	0.56
1:D:288:GLN:HA	1:D:291:THR:HG22	1.86	0.56
1:A:20:ALA:O	1:A:21:ALA:HB3	2.05	0.56
1:C:128:ASP:O	1:C:130:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLY:HA3	1:A:236:TYR:CE1	2.41	0.55
1:A:394:MET:HG2	1:C:394:MET:CG	2.34	0.55
1:A:146:VAL:HB	1:A:354:ARG:HH22	1.71	0.55
1:A:429:VAL:HG22	1:D:423:ILE:O	2.06	0.55
1:D:295:ASN:HB3	1:D:298:ASP:HB2	1.87	0.55
1:D:453:GLU:HA	1:D:456:ARG:HD2	1.89	0.54
1:B:214:GLY:HA3	1:B:236:TYR:CE2	2.43	0.54
1:B:139:GLU:OE1	1:B:139:GLU:N	2.38	0.54
1:C:27:LEU:HD21	1:C:38:LYS:HD3	1.90	0.54
3:A:602:HEM:HMB2	3:A:602:HEM:HBB2	1.91	0.53
1:B:55:VAL:HG11	1:D:337:SER:HB2	1.90	0.53
3:C:602:HEM:HMC2	3:C:602:HEM:HBC2	1.89	0.53
1:A:215:TYR:OH	2:A:601:LLR:BR7	2.72	0.53
1:B:16:LYS:CD	1:D:409:PHE:HA	2.39	0.53
1:D:233:LYS:HE2	1:D:303:TRP:CE2	2.44	0.53
1:C:70:PRO:HG3	1:D:70:PRO:HD3	1.92	0.52
1:D:143:TRP:HB2	1:D:340:PRO:HD3	1.90	0.52
1:A:156:ARG:NH1	1:A:300:THR:OG1	2.43	0.52
1:A:75:HIS:HA	1:A:115:THR:O	2.10	0.52
1:B:156:ARG:NH2	1:B:439:ASN:OD1	2.25	0.52
1:D:42:ILE:HB	1:D:54:ASP:HB2	1.91	0.52
1:D:430:ARG:NH2	4:D:744:HOH:O	2.43	0.52
1:B:391:PRO:HG3	1:D:69:ILE:HG22	1.91	0.52
1:D:415:GLN:NE2	4:D:722:HOH:O	2.34	0.52
1:C:70:PRO:HD3	1:D:70:PRO:HG3	1.92	0.51
1:A:263:ARG:NH1	4:A:729:HOH:O	2.41	0.51
1:A:171:ASN:HD21	1:B:11:GLN:HE21	1.59	0.51
1:A:124:ASP:O	1:A:130:ARG:NH2	2.43	0.51
1:C:431:ARG:HD2	1:D:37:ASP:HB3	1.92	0.51
1:B:295:ASN:HB3	1:B:298:ASP:HB2	1.93	0.51
1:B:405:TYR:H	1:C:163:SER:HB3	1.75	0.51
1:C:37:ASP:HB3	1:D:431:ARG:HD2	1.93	0.51
1:C:174:THR:HB	1:C:176:LEU:HD12	1.93	0.51
1:B:483:THR:HG22	1:B:490:GLY:HA3	1.94	0.50
1:D:50:LEU:HD12	1:D:51:LEU:H	1.76	0.50
1:A:288:GLN:HA	1:A:291:THR:HG22	1.93	0.50
1:D:392:MET:HE3	1:D:394:MET:HE3	1.92	0.50
1:A:75:HIS:CE1	1:A:116:VAL:HG22	2.47	0.50
1:A:386:TYR:OH	1:A:412:PRO:O	2.27	0.50
1:B:91:ILE:HG21	1:B:313:VAL:HG22	1.92	0.50
1:B:301:LYS:NZ	1:B:438:ASP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:HB2	1:A:430:ARG:HG2	1.94	0.49
1:B:448:VAL:HA	1:B:456:ARG:HH21	1.78	0.49
1:B:239:ASP:OD1	1:B:278:THR:OG1	2.31	0.49
1:C:66:ARG:HA	1:D:364:HIS:CD2	2.48	0.49
1:A:39:LEU:HA	1:B:160:LEU:HD21	1.95	0.49
1:B:233:LYS:NZ	4:B:715:HOH:O	2.33	0.49
1:B:468:LYS:HD3	1:B:500:TYR:HB3	1.94	0.49
3:B:602:HEM:HBB2	3:B:602:HEM:HMB2	1.95	0.49
1:D:226:ASN:ND2	4:D:753:HOH:O	2.46	0.49
1:A:64:PHE:HA	1:A:67:GLU:HG3	1.95	0.49
1:B:486:HIS:HB3	1:B:489:TYR:HB2	1.95	0.48
1:C:13:GLN:NE2	1:D:471:GLN:OE1	2.46	0.48
1:C:137:TYR:O	1:C:380:ARG:HD3	2.14	0.48
1:D:214:GLY:HA3	1:D:236:TYR:CE2	2.49	0.48
1:C:216:GLY:O	1:C:218:HIS:N	2.40	0.48
1:A:137:TYR:O	1:A:380:ARG:HD3	2.13	0.48
1:D:430:ARG:HG2	1:D:431:ARG:N	2.27	0.48
1:D:137:TYR:HB3	1:D:380:ARG:HG3	1.96	0.48
1:D:239:ASP:OD2	1:D:276:SER:OG	2.25	0.48
1:A:236:TYR:HA	1:A:278:THR:O	2.14	0.48
1:C:156:ARG:CZ	1:C:437:ASP:HB2	2.44	0.48
1:B:255:GLN:NE2	4:B:729:HOH:O	2.36	0.47
1:C:11:GLN:NE2	1:D:173:GLN:OE1	2.47	0.47
1:C:154:PHE:CE1	1:C:199:LEU:HD12	2.48	0.47
1:C:360:ASP:CG	1:D:66:ARG:HH12	2.23	0.47
1:B:16:LYS:HD2	1:D:409:PHE:HA	1.96	0.47
1:A:27:LEU:HD21	1:A:38:LYS:HD3	1.95	0.47
1:A:380:ARG:NE	4:A:742:HOH:O	2.46	0.47
1:A:216:GLY:O	1:A:218:HIS:N	2.43	0.47
1:A:368:PRO:HG2	1:A:391:PRO:HD2	1.95	0.47
1:C:358:TYR:HB2	1:C:359:PRO:HD3	1.96	0.47
1:A:66:ARG:HH12	1:B:360:ASP:CG	2.22	0.47
1:A:101:GLU:HB3	4:A:838:HOH:O	2.15	0.46
1:C:433:ASN:ND2	4:C:743:HOH:O	2.46	0.46
1:A:113:PHE:CD1	1:A:209:HIS:HB3	2.50	0.46
1:B:83:GLY:HA3	1:B:317:VAL:O	2.15	0.46
1:C:85:PHE:HB2	1:C:316:LEU:HD23	1.97	0.46
1:D:47:ARG:NH2	4:D:762:HOH:O	2.48	0.46
1:C:448:VAL:O	1:C:456:ARG:NH2	2.49	0.46
1:D:282:GLN:HG3	1:D:310:LEU:HD23	1.97	0.46
1:D:216:GLY:O	1:D:218:HIS:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD12	1:A:51:LEU:H	1.81	0.45
1:A:77:LYS:NZ	1:A:124:ASP:OD1	2.48	0.45
1:A:119:GLU:CD	1:A:119:GLU:H	2.24	0.45
1:C:146:VAL:HB	1:C:354:ARG:HH22	1.81	0.45
1:D:350:MET:HE3	3:D:602:HEM:HAB	1.97	0.45
1:A:296:PRO:HD2	1:B:47:ARG:HH12	1.81	0.45
1:B:44:VAL:O	1:B:48:GLY:HA3	2.16	0.45
1:B:479:VAL:O	1:B:483:THR:HG23	2.16	0.45
1:D:488:ASP:O	1:D:492:HIS:HB2	2.16	0.45
1:A:84:TYR:CD1	1:A:106:LYS:HD3	2.51	0.45
1:B:415:GLN:O	1:D:36:GLY:HA2	2.17	0.45
1:D:358:TYR:HB2	1:D:359:PRO:HD3	1.98	0.45
1:D:284:MET:HE2	1:D:308:TYR:CZ	2.52	0.45
1:A:55:VAL:HG11	1:C:337:SER:HB2	1.98	0.45
1:B:81:ALA:HB3	1:B:318:LEU:HD13	1.99	0.45
1:C:49:PRO:HD3	1:D:425:TYR:CZ	2.52	0.45
1:A:83:GLY:HA3	1:A:317:VAL:O	2.17	0.45
1:A:288:GLN:NE2	4:A:712:HOH:O	2.32	0.45
1:C:154:PHE:HE1	1:C:199:LEU:HD12	1.81	0.45
1:A:263:ARG:NH2	4:A:753:HOH:O	2.49	0.45
1:C:329:VAL:O	1:C:332:ILE:HG22	2.17	0.44
1:A:16:LYS:O	1:A:19:ARG:HB3	2.18	0.44
1:B:16:LYS:HD3	1:D:409:PHE:HA	1.98	0.44
1:B:25:ASP:OD2	1:D:382:ARG:NH2	2.50	0.44
1:B:275:PRO:HG2	1:B:318:LEU:HB2	1.99	0.44
1:B:362:HIS:NE2	3:B:602:HEM:O1A	2.47	0.44
1:B:36:GLY:HA2	1:D:415:GLN:O	2.17	0.44
1:B:329:VAL:O	1:B:332:ILE:HG22	2.17	0.44
1:D:91:ILE:HG21	1:D:313:VAL:HG22	2.00	0.44
1:B:351:LEU:O	1:B:355:LEU:HG	2.18	0.44
1:B:440:VAL:HG11	1:B:484:GLU:HG2	2.00	0.44
1:C:444:ARG:NH2	1:C:484:GLU:O	2.46	0.44
1:A:235:HIS:HB2	1:A:280:TYR:HB2	2.00	0.43
1:D:146:VAL:HG22	1:D:334:PHE:HB3	2.00	0.43
1:A:333:ALA:HB1	1:A:362:HIS:CE1	2.52	0.43
1:C:14:HIS:O	1:C:18:GLN:HG2	2.18	0.43
1:C:218:HIS:CE1	1:C:299:LEU:HD22	2.53	0.43
1:A:213:ASN:OD1	1:A:238:THR:HG22	2.18	0.43
1:B:118:GLY:O	4:B:701:HOH:O	2.21	0.43
1:D:44:VAL:O	1:D:48:GLY:HA3	2.18	0.43
1:A:329:VAL:O	1:A:332:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:CE2	1:A:294:PHE:HB2	2.54	0.43
1:D:167:SER:HA	1:D:181:MET:HE2	2.01	0.43
1:D:335:ASP:HB2	1:D:338:ASN:ND2	2.34	0.43
1:A:221:LYS:HB3	1:A:344:GLU:HB2	1.99	0.43
1:B:449:ASN:OD1	1:B:449:ASN:N	2.52	0.43
1:D:169:LYS:HB3	1:D:170:ARG:H	1.72	0.43
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.91	0.42
1:B:75:HIS:CE1	1:B:116:VAL:HG22	2.54	0.42
1:C:350:MET:O	1:C:354:ARG:HG3	2.19	0.42
1:D:177:LYS:HE3	4:D:970:HOH:O	2.18	0.42
1:A:18:GLN:HB2	4:A:739:HOH:O	2.20	0.42
1:A:166:HIS:NE2	1:B:67:GLU:OE1	2.40	0.42
1:C:136:PHE:HB2	1:C:143:TRP:HB3	2.00	0.42
1:C:42:ILE:HG22	1:C:51:LEU:HD12	2.01	0.42
1:C:93:LYS:HD2	1:C:94:TYR:CE1	2.54	0.42
1:D:259:ASP:HB3	1:D:262:ILE:HD12	2.02	0.42
1:A:296:PRO:HD2	1:B:47:ARG:NH1	2.34	0.42
1:C:50:LEU:HD12	1:C:51:LEU:H	1.85	0.42
1:C:217:SER:HB3	1:C:299:LEU:HD11	2.01	0.42
1:C:407:ASN:HD21	1:C:411:ALA:HB3	1.85	0.42
1:D:232:CYS:HA	1:D:282:GLN:O	2.20	0.42
1:B:66:ARG:HD3	1:D:368:PRO:HG3	2.01	0.42
1:D:301:LYS:NZ	4:D:770:HOH:O	2.51	0.42
1:B:131:GLY:HA2	1:B:148:ASN:HB3	2.01	0.42
1:C:121:GLY:CA	1:D:119:GLU:HG2	2.50	0.42
1:A:273:LYS:NZ	4:A:769:HOH:O	2.53	0.42
1:A:364:HIS:CG	1:B:66:ARG:HG2	2.55	0.42
1:C:295:ASN:HB3	1:C:298:ASP:HB2	2.02	0.41
1:A:415:GLN:O	1:C:36:GLY:HA2	2.20	0.41
1:B:407:ASN:HD21	1:B:411:ALA:HB3	1.85	0.41
1:C:75:HIS:CE1	1:C:116:VAL:HG22	2.55	0.41
1:C:333:ALA:HB1	1:C:362:HIS:CE1	2.54	0.41
1:B:416:PRO:HD2	4:B:1081:HOH:O	2.19	0.41
1:B:180:ASP:OD2	1:B:471:GLN:HG3	2.20	0.41
1:C:93:LYS:HE3	1:C:93:LYS:HB3	1.78	0.41
1:C:452:ASN:O	1:C:456:ARG:HG3	2.20	0.41
1:B:64:PHE:HA	1:B:67:GLU:HG3	2.03	0.41
1:C:255:GLN:HG3	1:D:251:ALA:O	2.21	0.41
1:D:110:ALA:HB3	1:D:135:LYS:HB3	2.03	0.41
1:D:237:LYS:HE2	1:D:310:LEU:HD11	2.02	0.41
1:A:19:ARG:O	1:A:22:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LYS:O	1:C:101:GLU:HB2	2.20	0.41
1:A:193:LEU:HD21	1:A:481:ASN:HB3	2.03	0.41
1:A:337:SER:HB2	1:C:55:VAL:HG21	2.03	0.41
1:D:184:ASP:O	1:D:188:LEU:HG	2.21	0.41
1:A:403:ASN:O	1:D:166:HIS:ND1	2.54	0.41
1:A:16:LYS:HG3	1:C:409:PHE:HA	2.02	0.41
1:A:119:GLU:HG2	1:B:121:GLY:CA	2.51	0.41
1:C:42:ILE:HG12	1:D:431:ARG:HG2	2.03	0.41
1:C:358:TYR:HA	1:C:361:THR:HG22	2.03	0.41
1:B:407:ASN:ND2	1:B:411:ALA:HB3	2.36	0.40
1:A:173:GLN:NE2	1:B:11:GLN:OE1	2.54	0.40
1:C:170:ARG:HD2	1:C:175:HIS:CE1	2.56	0.40
1:B:144:ASP:HB2	1:B:335:ASP:O	2.21	0.40
1:B:288:GLN:HA	1:B:291:THR:HG22	2.03	0.40
1:B:358:TYR:HB2	1:B:359:PRO:HD3	2.02	0.40
1:D:376:ASN:N	4:D:701:HOH:O	2.23	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	496/527 (94%)	473 (95%)	23 (5%)	0	100	100
1	B	496/527 (94%)	474 (96%)	22 (4%)	0	100	100
1	C	497/527 (94%)	476 (96%)	21 (4%)	0	100	100
1	D	496/527 (94%)	473 (95%)	23 (5%)	0	100	100
All	All	1985/2108 (94%)	1896 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	427/451 (95%)	412 (96%)	15 (4%)	32	43
1	B	425/451 (94%)	412 (97%)	13 (3%)	35	48
1	C	428/451 (95%)	415 (97%)	13 (3%)	36	49
1	D	426/451 (94%)	412 (97%)	14 (3%)	33	45
All	All	1706/1804 (95%)	1651 (97%)	55 (3%)	34	47

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	19	ARG
1	A	23	LYS
1	A	41	VAL
1	A	44	VAL
1	A	128	ASP
1	A	138	THR
1	A	232	CYS
1	A	247	VAL
1	A	248	GLU
1	A	255	GLN
1	A	290	GLU
1	A	301	LYS
1	A	394	MET
1	A	424	GLN
1	B	16	LYS
1	B	18	GLN
1	B	19	ARG
1	B	41	VAL
1	B	44	VAL
1	B	119	GLU
1	B	138	THR
1	B	290	GLU
1	B	305	HIS

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Mol	Chain	Res	Type
1	B	306	LYS
1	B	377	CYS
1	B	449	ASN
1	B	468	LYS
1	C	11	GLN
1	C	19	ARG
1	C	23	LYS
1	C	41	VAL
1	C	44	VAL
1	C	119	GLU
1	C	128	ASP
1	C	199	LEU
1	C	236	TYR
1	C	291	THR
1	C	377	CYS
1	C	394	MET
1	C	426	SER
1	D	11	GLN
1	D	22	GLN
1	D	41	VAL
1	D	44	VAL
1	D	74	VAL
1	D	119	GLU
1	D	128	ASP
1	D	138	THR
1	D	146	VAL
1	D	248	GLU
1	D	307	ASP
1	D	377	CYS
1	D	380	ARG
1	D	454	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	173	GLN
1	A	352	GLN
1	B	13	GLN
1	B	168	GLN
1	B	244	ASN
1	B	305	HIS

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Mol	Chain	Res	Type
1	C	173	GLN
1	C	211	HIS
1	C	255	GLN
1	D	11	GLN
1	D	244	ASN
1	D	255	GLN
1	D	338	ASN
1	D	424	GLN
1	D	494	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	LLR	D	601	-	14,18,18	1.60	3 (21%)	16,23,23	0.88	1 (6%)
3	HEM	C	602	1	50,50,50	1.46	9 (18%)	67,82,82	1.24	7 (10%)
2	LLR	A	601	-	14,18,18	1.57	2 (14%)	16,23,23	0.80	0
2	LLR	B	601	-	14,18,18	1.58	3 (21%)	16,23,23	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LLR	C	601	-	14,18,18	1.62	2 (14%)	16,23,23	0.72	0
3	HEM	B	602	1	50,50,50	1.48	8 (16%)	67,82,82	1.16	5 (7%)
3	HEM	D	602	1	50,50,50	1.45	7 (14%)	67,82,82	1.17	8 (11%)
3	HEM	A	602	1	50,50,50	1.43	7 (14%)	67,82,82	1.22	6 (8%)

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	LLR	D	601	-	-	6/11/14/14	0/1/1/1
3	HEM	C	602	1	-	2/14/54/54	-
2	LLR	A	601	-	-	6/11/14/14	0/1/1/1
2	LLR	B	601	-	-	5/11/14/14	0/1/1/1
2	LLR	C	601	-	-	6/11/14/14	0/1/1/1
3	HEM	B	602	1	-	2/14/54/54	-
3	HEM	D	602	1	-	2/14/54/54	-
3	HEM	A	602	1	-	4/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	LLR	C04-N14	4.38	1.50	1.41
2	A	601	LLR	C04-N14	4.26	1.50	1.41
2	B	601	LLR	C04-N14	4.18	1.50	1.41
2	D	601	LLR	C04-N14	4.13	1.50	1.41
3	B	602	HEM	FE-ND	3.99	2.07	1.94
3	C	602	HEM	FE-NA	3.87	2.07	1.95
3	A	602	HEM	FE-NB	3.81	2.06	1.94
3	C	602	HEM	FE-ND	3.69	2.06	1.94
3	D	602	HEM	FE-NC	3.57	2.07	1.95
3	B	602	HEM	FE-NA	3.56	2.06	1.95
3	A	602	HEM	FE-NA	3.44	2.06	1.95
3	D	602	HEM	FE-NB	3.29	2.05	1.94
3	D	602	HEM	FE-ND	3.28	2.05	1.94
3	B	602	HEM	FE-NC	3.22	2.05	1.95
3	D	602	HEM	FE-NA	3.22	2.05	1.95
3	D	602	HEM	CAC-C3C	3.18	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	FE-NB	3.15	2.04	1.94
3	C	602	HEM	FE-NB	3.15	2.04	1.94
3	A	602	HEM	FE-NC	3.14	2.05	1.95
3	D	602	HEM	CAB-C3B	3.09	1.55	1.47
3	C	602	HEM	CAC-C3C	3.07	1.55	1.47
3	C	602	HEM	FE-NC	3.06	2.05	1.95
3	B	602	HEM	CAC-C3C	3.03	1.55	1.47
3	A	602	HEM	CAB-C3B	3.02	1.55	1.47
3	C	602	HEM	CAB-C3B	2.97	1.55	1.47
3	A	602	HEM	CAC-C3C	2.97	1.55	1.47
3	B	602	HEM	CAB-C3B	2.96	1.55	1.47
3	A	602	HEM	FE-ND	2.82	2.03	1.94
2	D	601	LLR	N09-N10	2.26	1.44	1.41
2	D	601	LLR	BR7-C05	2.24	1.94	1.89
2	B	601	LLR	BR7-C05	2.21	1.94	1.89
3	B	602	HEM	CMC-C2C	2.20	1.55	1.50
2	B	601	LLR	N09-N10	2.16	1.44	1.41
3	B	602	HEM	CMB-C2B	2.13	1.55	1.50
3	D	602	HEM	CMB-C2B	2.11	1.55	1.50
2	C	601	LLR	BR7-C05	2.11	1.94	1.89
2	A	601	LLR	BR7-C05	2.11	1.94	1.89
3	C	602	HEM	CMC-C2C	2.09	1.55	1.50
3	A	602	HEM	CMC-C2C	2.08	1.55	1.50
3	C	602	HEM	CMB-C2B	2.08	1.55	1.50
3	C	602	HEM	CMD-C2D	2.01	1.54	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	HEM	C4D-ND-C1D	2.82	108.54	105.21
3	A	602	HEM	C2A-C1A-NA	-2.79	107.06	110.15
3	A	602	HEM	C4D-ND-C1D	2.66	108.36	105.21
3	C	602	HEM	C1B-NB-C4B	2.63	108.32	105.21
3	C	602	HEM	C4D-ND-C1D	2.56	108.24	105.21
3	A	602	HEM	C3D-C4D-ND	-2.52	107.41	110.17
3	D	602	HEM	C1B-NB-C4B	2.51	108.19	105.21
3	B	602	HEM	C4D-ND-C1D	2.51	108.18	105.21
3	A	602	HEM	CAD-CBD-CGD	-2.47	107.10	113.67
3	B	602	HEM	C1B-NB-C4B	2.44	108.10	105.21
3	D	602	HEM	C3D-C4D-ND	-2.44	107.50	110.17
3	D	602	HEM	C3B-C2B-C1B	2.40	108.21	106.41
3	C	602	HEM	C3D-C4D-ND	-2.39	107.55	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	HEM	C2A-C1A-NA	-2.38	107.51	110.15
3	B	602	HEM	C2A-C1A-NA	-2.32	107.58	110.15
3	B	602	HEM	CAD-CBD-CGD	-2.27	107.64	113.67
3	B	602	HEM	C3D-C4D-ND	-2.26	107.69	110.17
3	C	602	HEM	CAD-CBD-CGD	-2.24	107.71	113.67
3	A	602	HEM	C3B-C2B-C1B	2.20	108.06	106.41
3	C	602	HEM	C3B-C2B-C1B	2.19	108.06	106.41
3	A	602	HEM	C1B-NB-C4B	2.19	107.80	105.21
3	C	602	HEM	C3B-C4B-NB	-2.13	107.94	109.47
3	D	602	HEM	C2A-C1A-NA	-2.10	107.83	110.15
3	D	602	HEM	CHD-C1D-ND	2.07	126.65	124.42
3	D	602	HEM	CAD-CBD-CGD	-2.07	108.18	113.67
3	D	602	HEM	C2D-C1D-ND	-2.04	107.55	109.90
2	D	601	LLR	C17-N14-C15	2.02	120.13	116.31

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	LLR	C16-C15-N14-C04
2	A	601	LLR	C16-C15-N14-C04
2	A	601	LLR	C18-C17-N14-C04
2	A	601	LLR	C16-C15-N14-C17
2	C	601	LLR	C16-C15-N14-C17
2	A	601	LLR	C18-C17-N14-C15
2	B	601	LLR	C16-C15-N14-C04
2	B	601	LLR	C16-C15-N14-C17
2	D	601	LLR	C02-C01-C08-N09
2	D	601	LLR	C06-C01-C08-N09
2	A	601	LLR	C05-C04-N14-C17
2	D	601	LLR	C18-C17-N14-C04
2	D	601	LLR	C05-C04-N14-C17
2	D	601	LLR	C18-C17-N14-C15
2	A	601	LLR	C03-C04-N14-C17
2	D	601	LLR	C03-C04-N14-C17
3	D	602	HEM	CAD-CBD-CGD-O2D
3	D	602	HEM	CAD-CBD-CGD-O1D
2	B	601	LLR	C01-C08-N09-N10
3	A	602	HEM	CAD-CBD-CGD-O2D
2	B	601	LLR	C03-C04-N14-C15
3	B	602	HEM	CAD-CBD-CGD-O2D
3	C	602	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	A	602	HEM	CAD-CBD-CGD-O1D
3	B	602	HEM	CAD-CBD-CGD-O1D
3	C	602	HEM	CAD-CBD-CGD-O1D
2	B	601	LLR	C05-C04-N14-C15
2	C	601	LLR	C03-C04-N14-C15
2	C	601	LLR	C03-C04-N14-C17
3	A	602	HEM	CAA-CBA-CGA-O1A
2	C	601	LLR	C05-C04-N14-C15
2	C	601	LLR	C05-C04-N14-C17
3	A	602	HEM	CAA-CBA-CGA-O2A

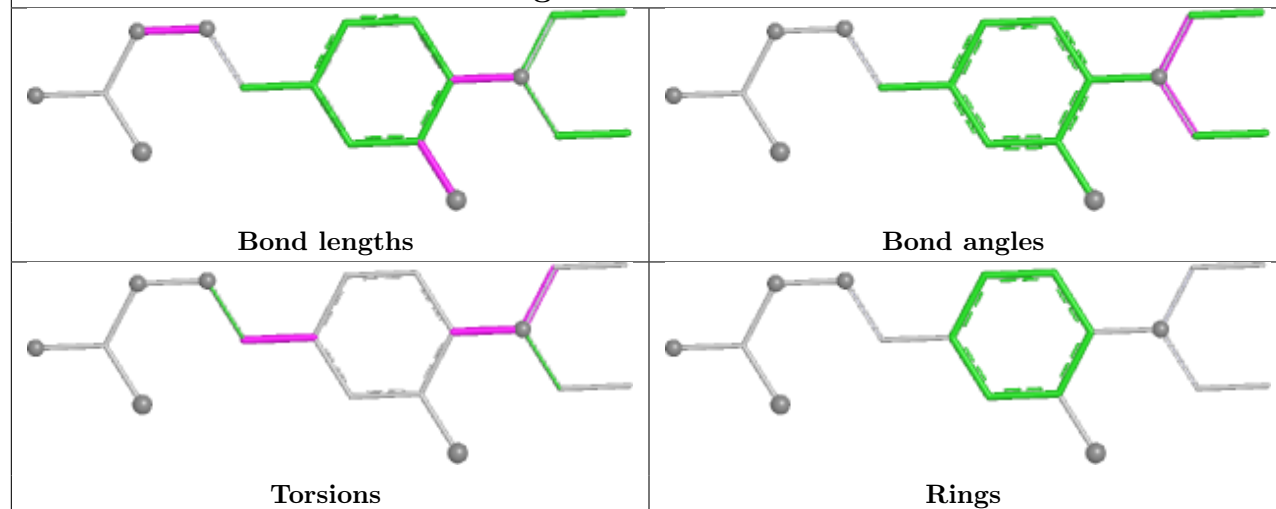
There are no ring outliers.

5 monomers are involved in 11 short contacts:

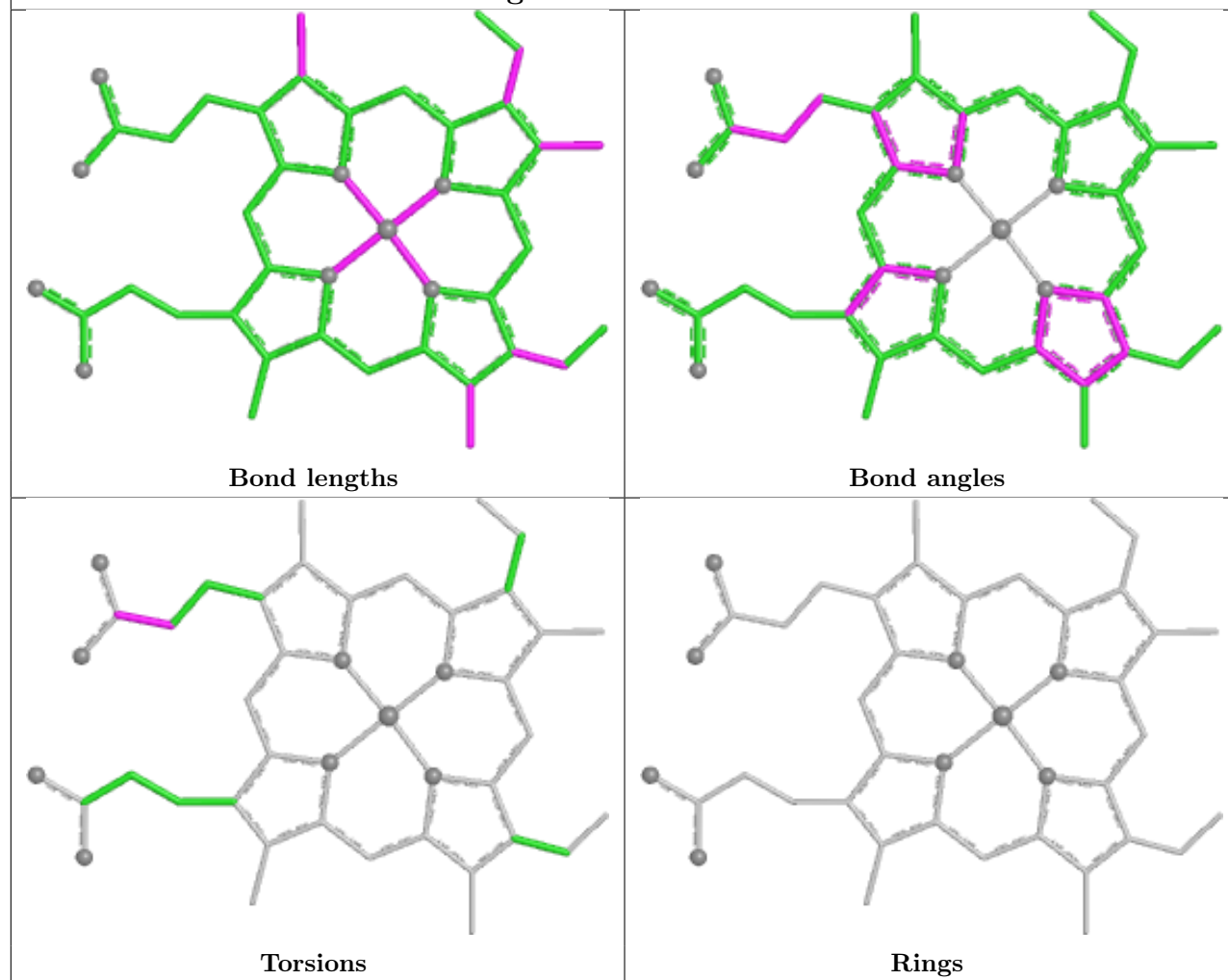
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	HEM	2	0
2	A	601	LLR	1	0
3	B	602	HEM	3	0
3	D	602	HEM	3	0
3	A	602	HEM	2	0

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.

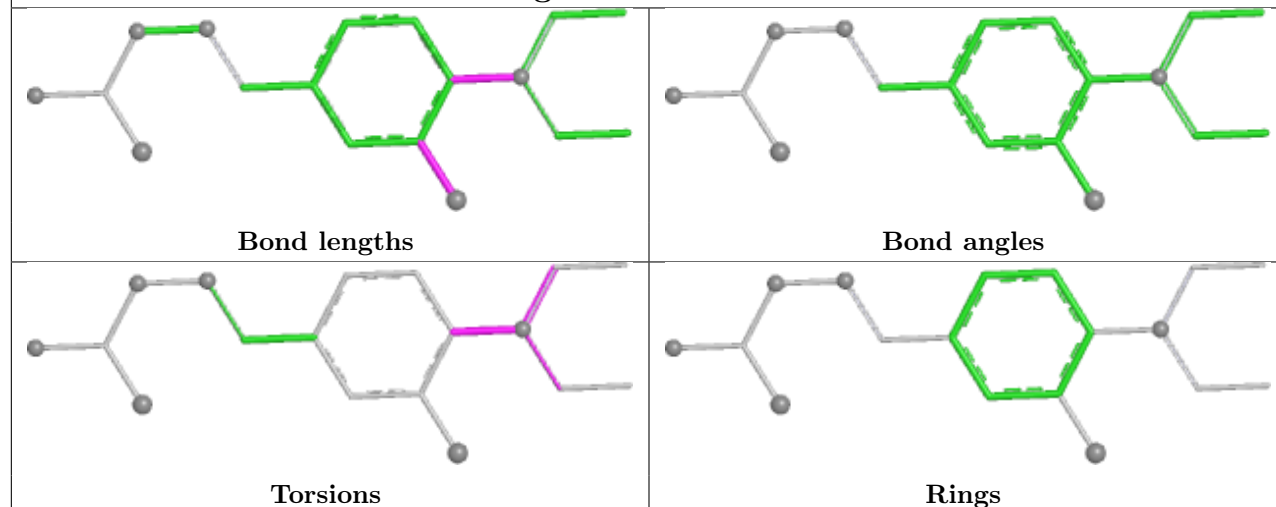
Ligand LLR D 601



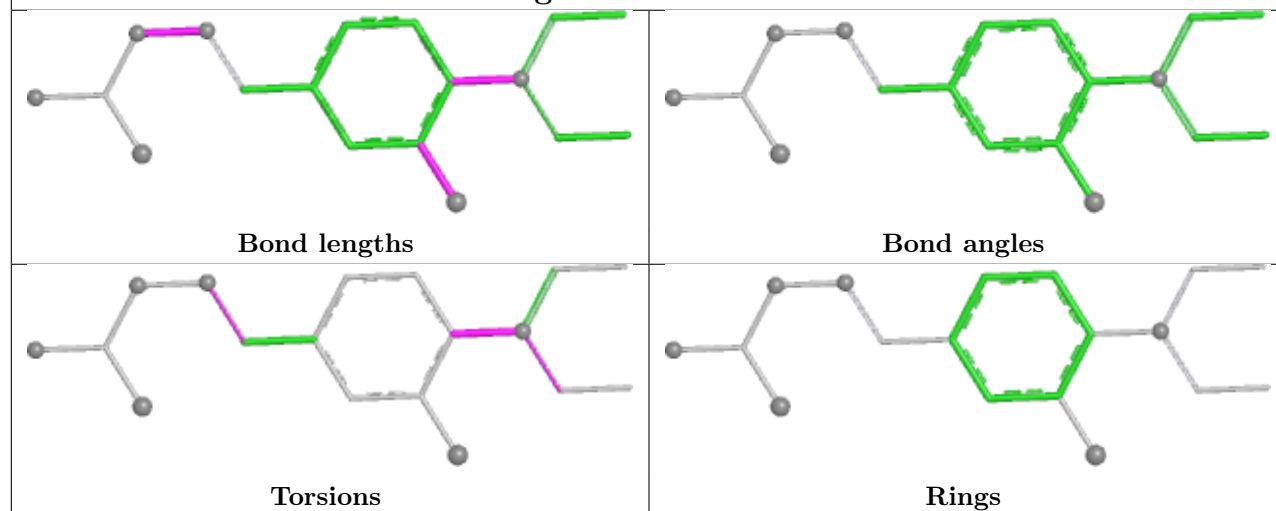
Ligand HEM C 602



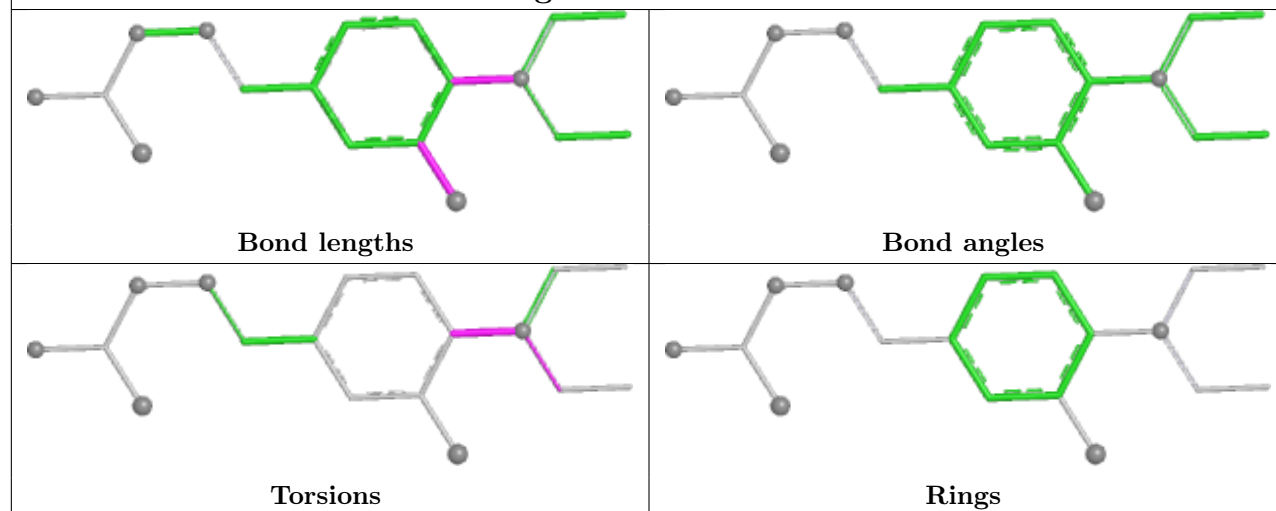
Ligand LLR A 601

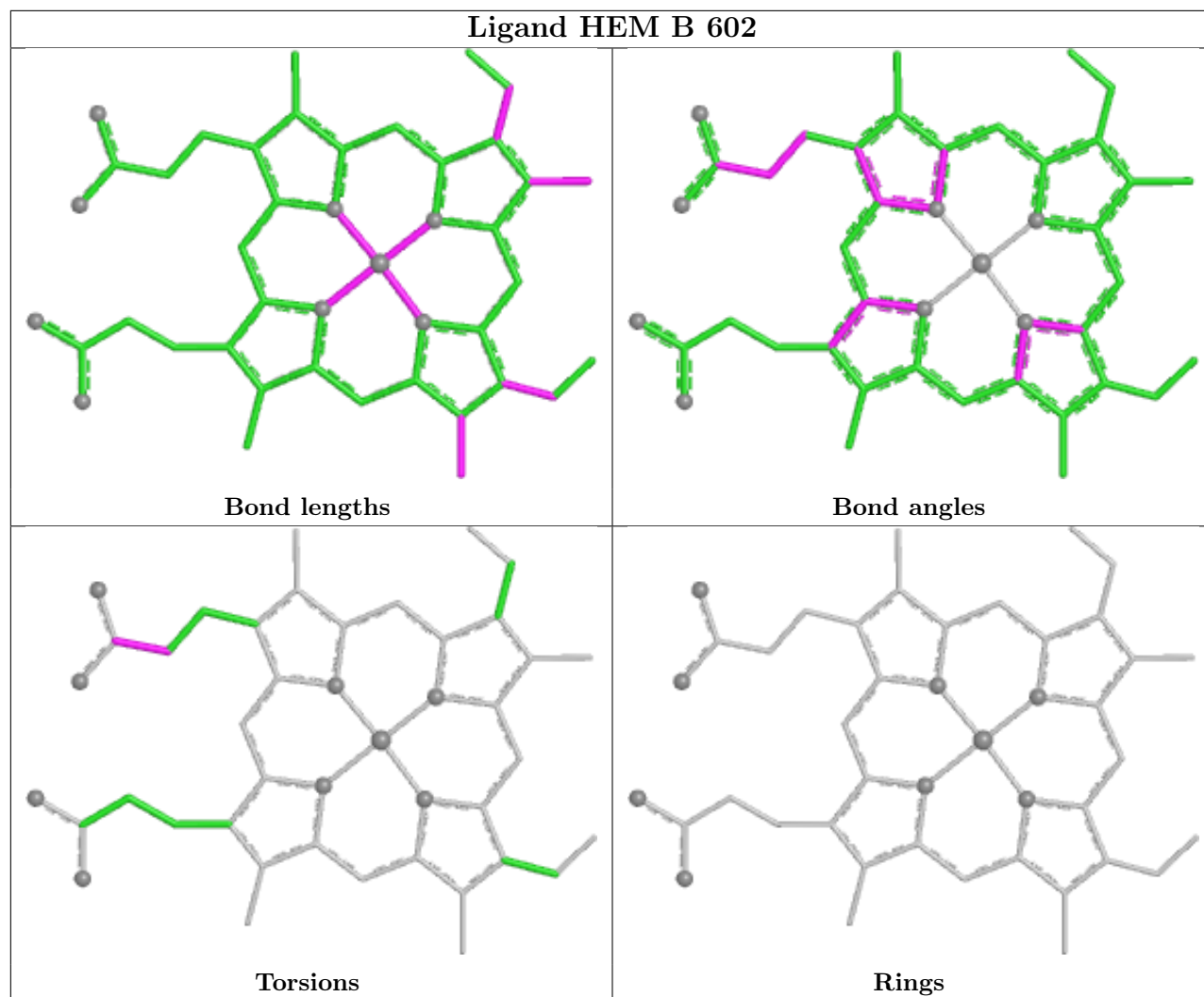


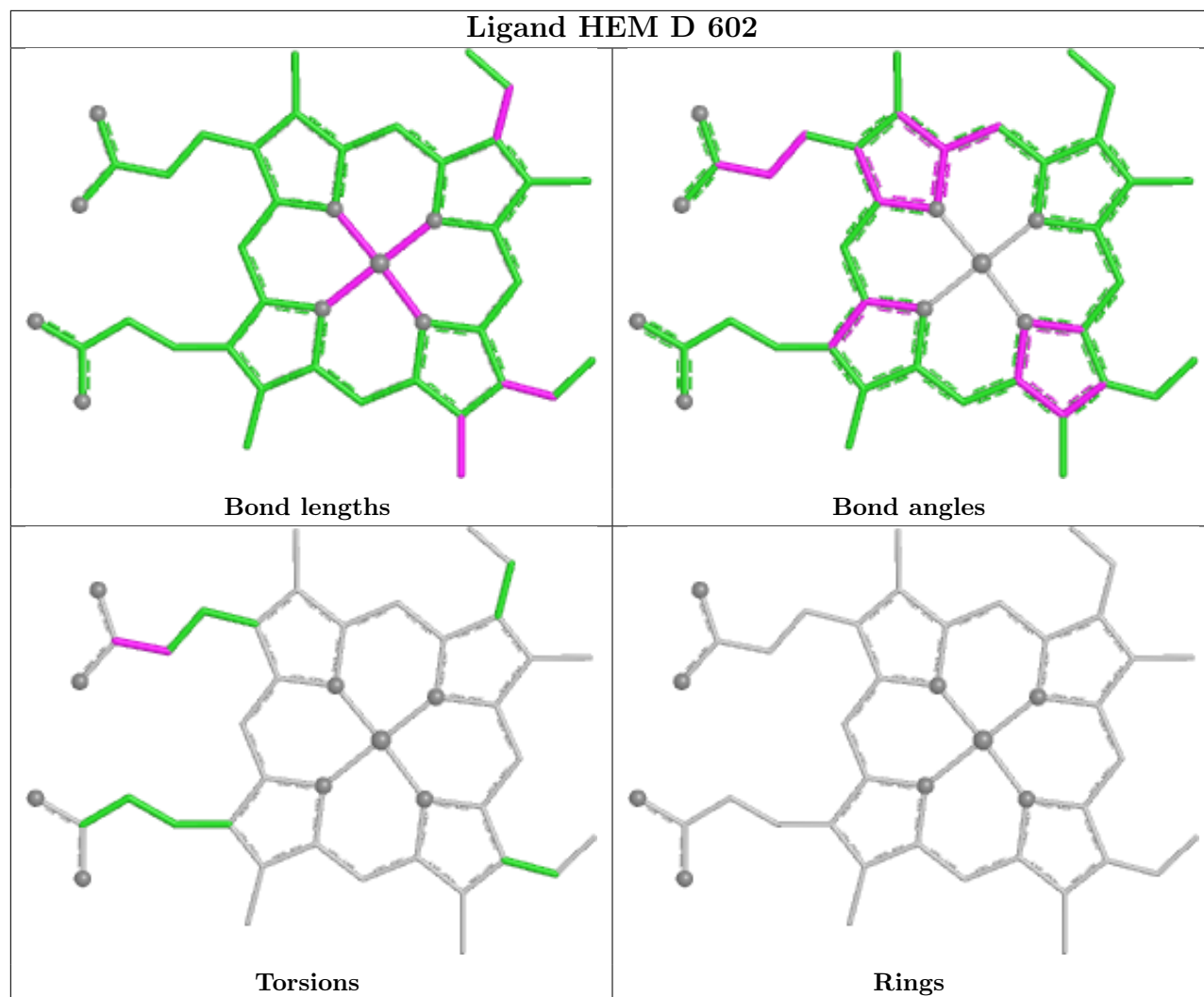
Ligand LLR B 601

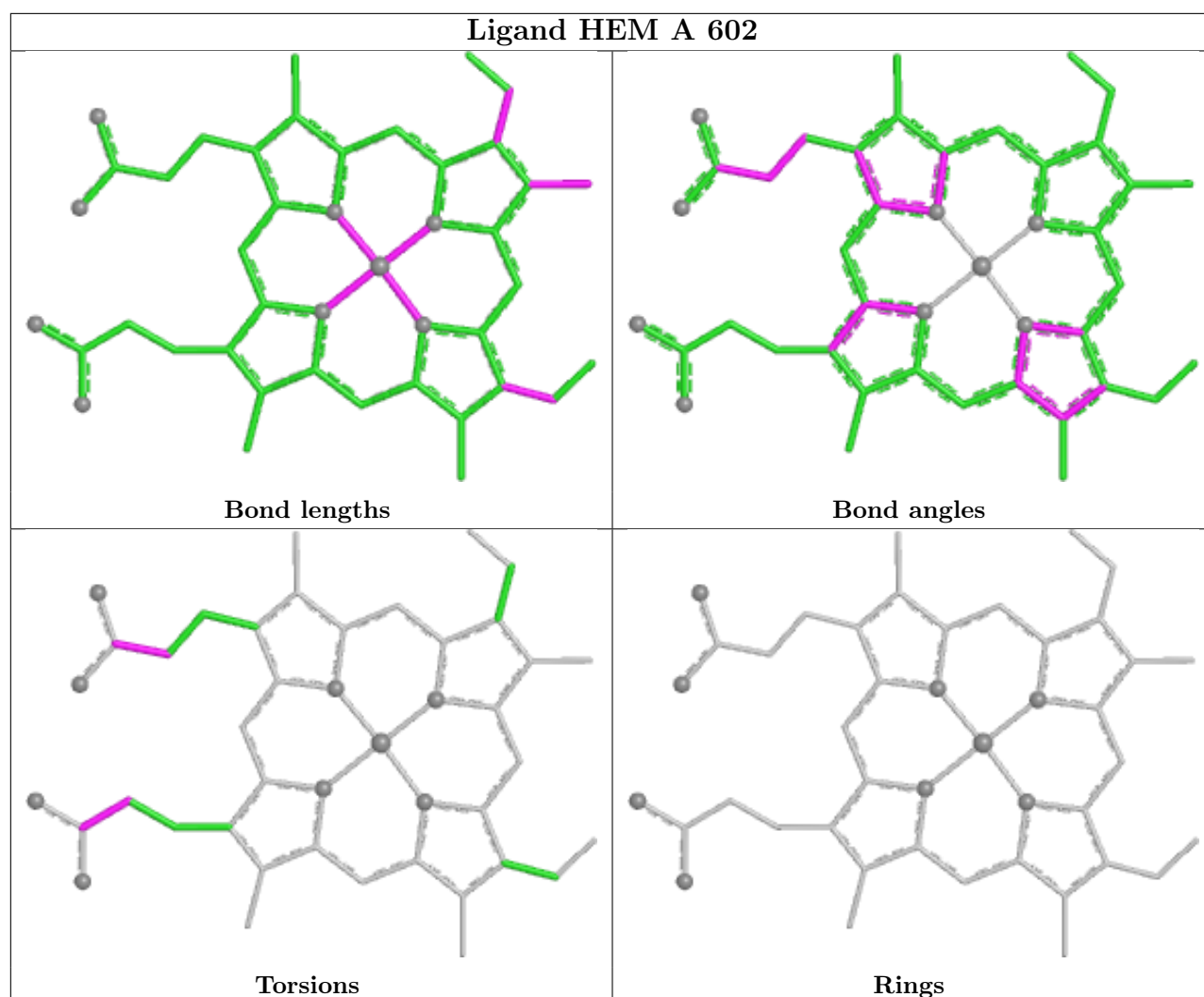


Ligand LLR C 601









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	498/527 (94%)	0.07	5 (1%) 79 77	16, 28, 47, 63	0
1	B	498/527 (94%)	0.17	4 (0%) 82 80	18, 29, 48, 63	0
1	C	499/527 (94%)	0.16	5 (1%) 79 77	18, 31, 47, 67	0
1	D	498/527 (94%)	0.17	5 (1%) 79 77	19, 31, 48, 58	0
All	All	1993/2108 (94%)	0.15	19 (0%) 79 77	16, 30, 47, 67	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	ALA	4.7
1	C	21	ALA	4.2
1	D	20	ALA	4.1
1	C	20	ALA	3.8
1	B	502	ALA	3.6
1	A	21	ALA	3.6
1	D	502	ALA	3.1
1	A	394	MET	2.9
1	A	502	ALA	2.8
1	A	5	ARG	2.8
1	D	21	ALA	2.6
1	B	198	PHE	2.6
1	D	19	ARG	2.4
1	A	20	ALA	2.3
1	C	502	ALA	2.3
1	C	448	VAL	2.2
1	C	490	GLY	2.2
1	D	470	ALA	2.2
1	B	17	GLU	2.1

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](#)

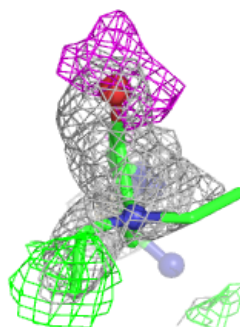
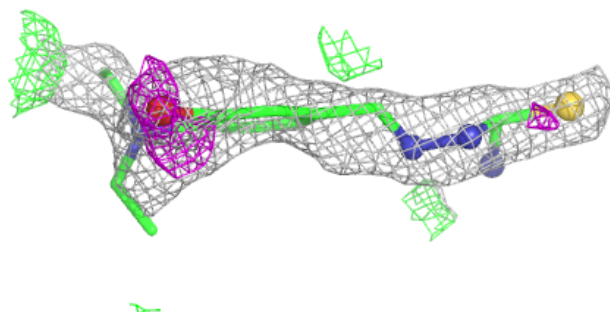
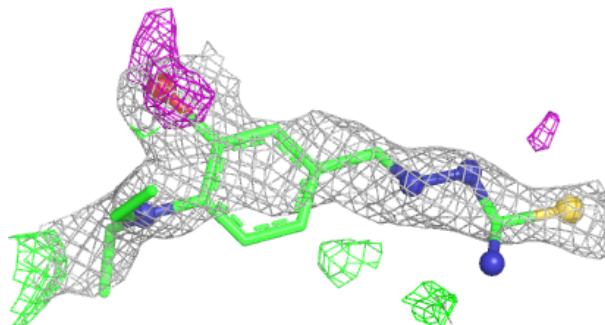
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LLR	C	601	18/18	0.68	0.21	57,64,79,108	0
2	LLR	A	601	18/18	0.73	0.19	43,58,76,97	0
2	LLR	B	601	18/18	0.74	0.18	43,59,71,102	0
2	LLR	D	601	18/18	0.74	0.21	60,74,85,105	0
3	HEM	B	602	43/43	0.94	0.09	14,24,29,37	0
3	HEM	C	602	43/43	0.94	0.08	18,24,29,42	0
3	HEM	D	602	43/43	0.94	0.09	18,25,30,43	0
3	HEM	A	602	43/43	0.95	0.08	17,23,28,42	0

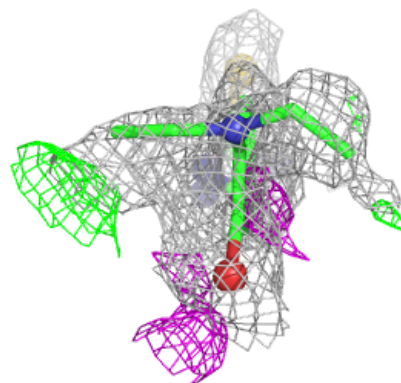
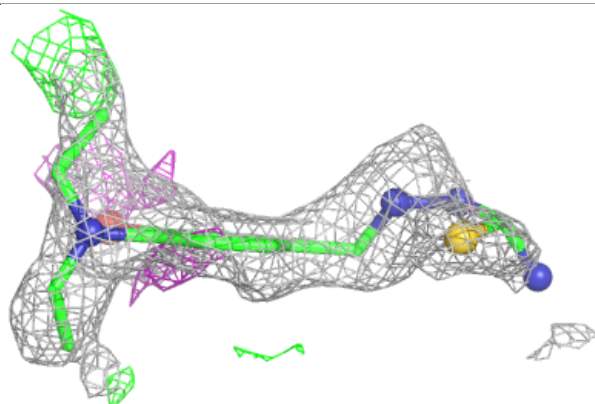
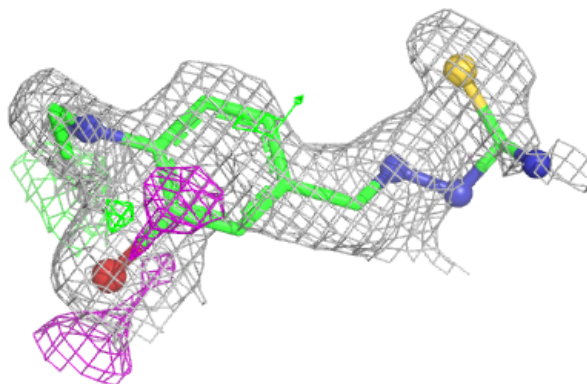
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LLR 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)

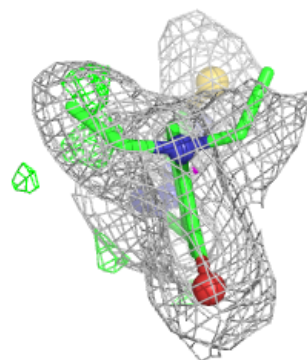
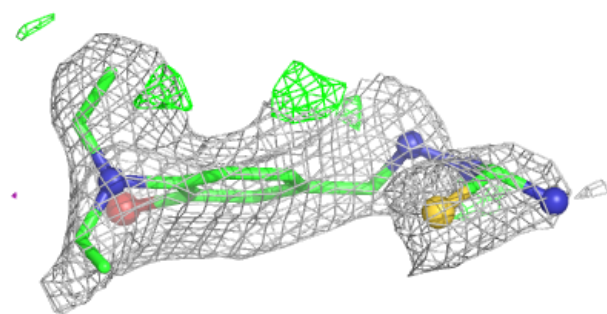
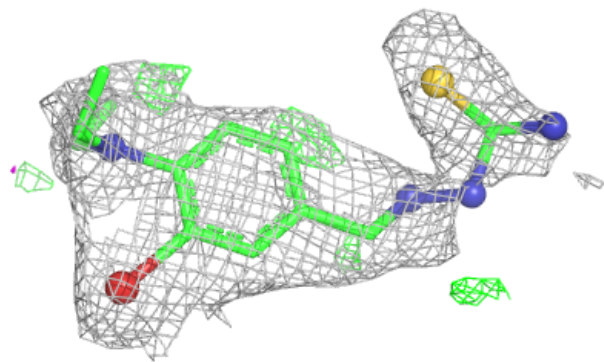
**Electron density around LLR A 601:**

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

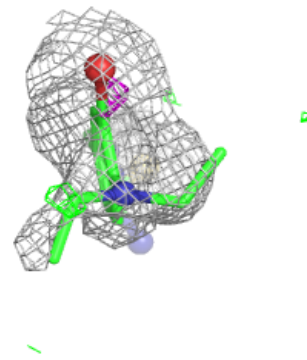
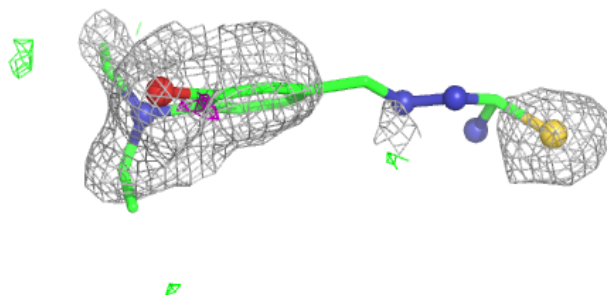
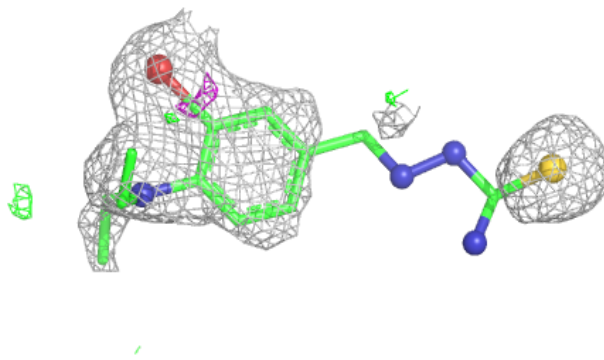


Electron density around LLR B 601:

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

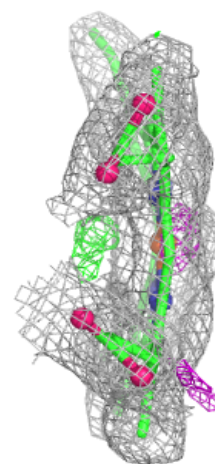
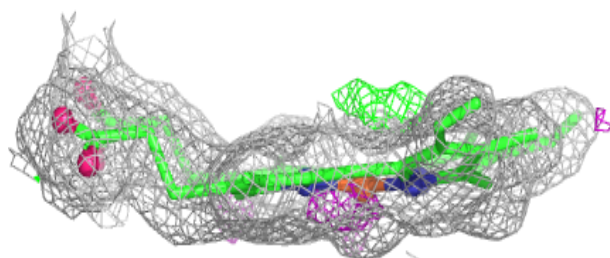
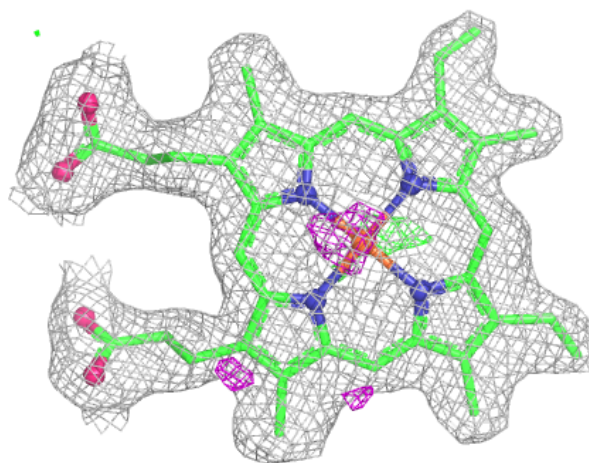
**Electron density around LLR D 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



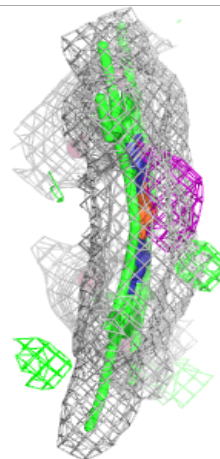
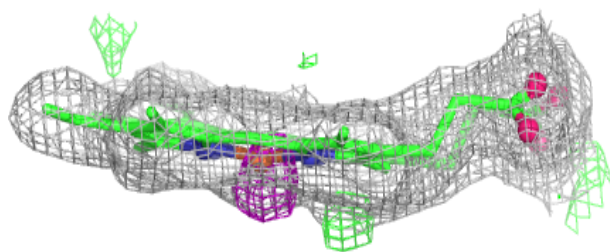
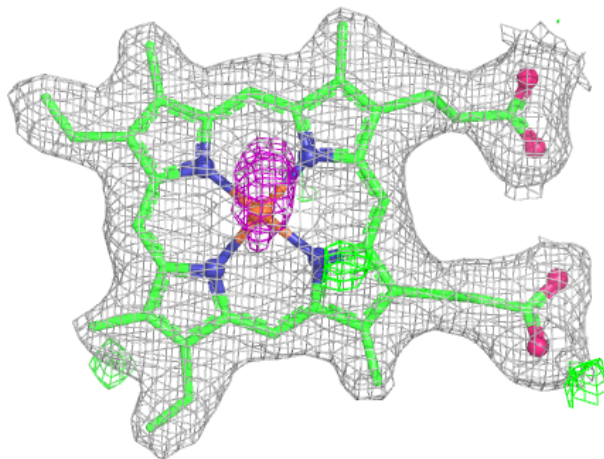
Electron density around HEM B 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



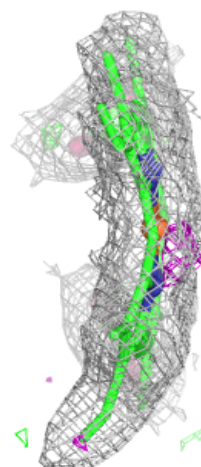
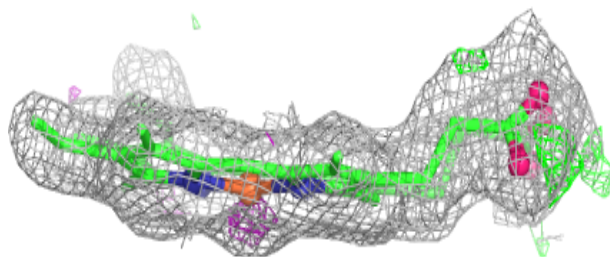
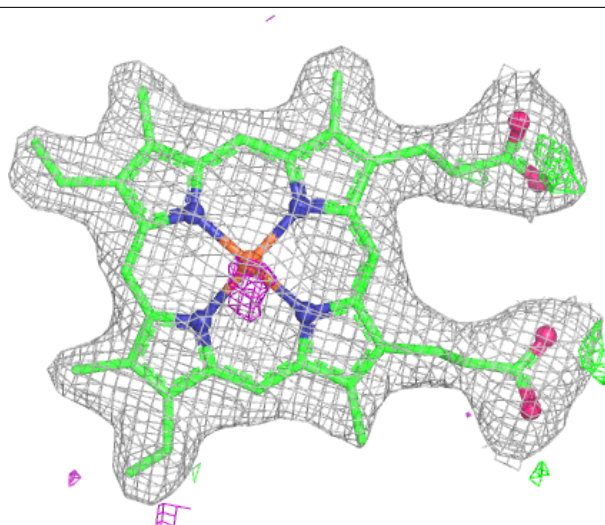
Electron density around HEM C 602:

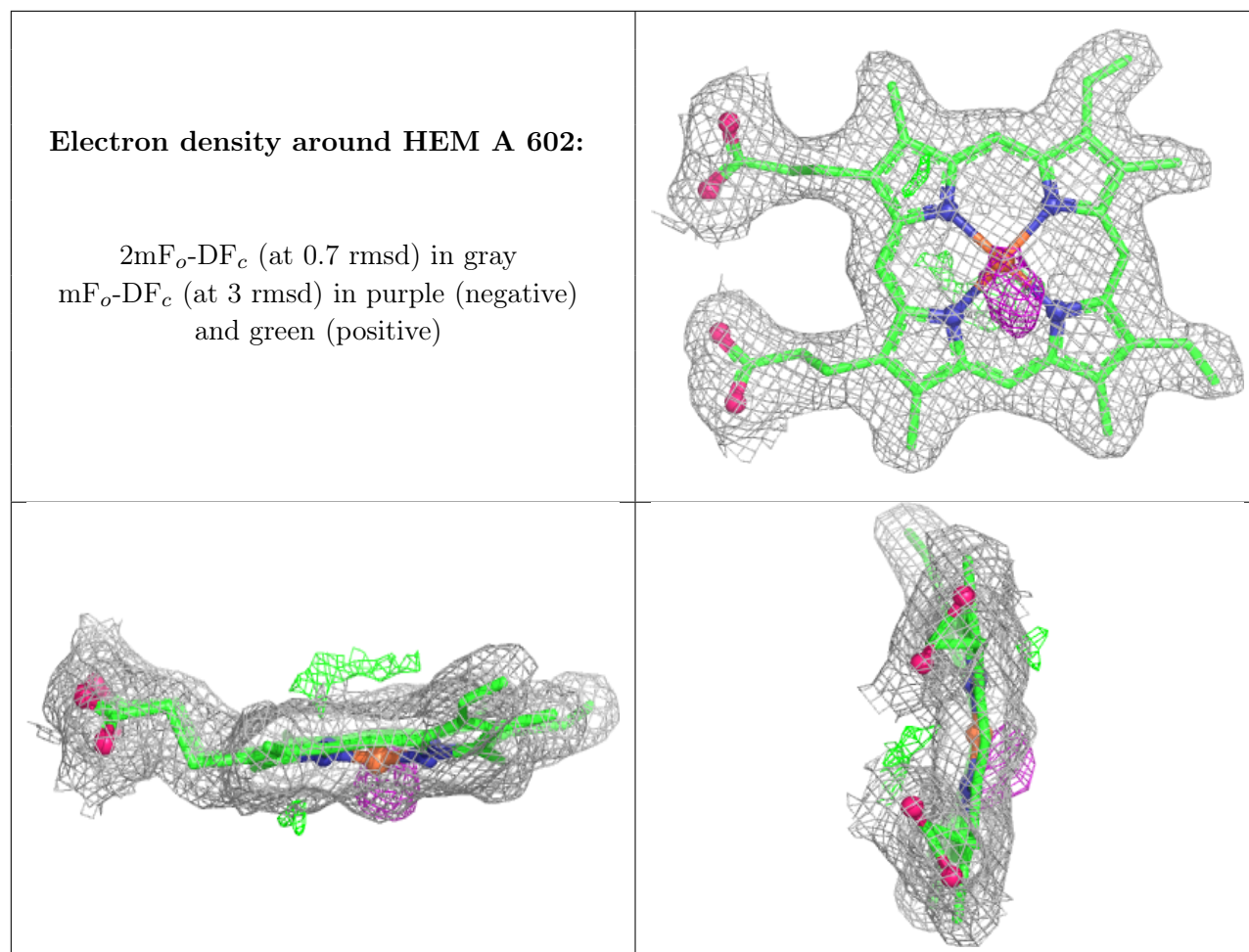
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.