



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:23 PM UTC

PDB ID : 7SNM / pdb_00007snm
Title : Lanosterol-bound P450 domain of the CYP51-ferredoxin fusion protein from *Methylococcus capsulatus*
Authors : Lepesheva, G.I.; Hargrove, T.; Wawrzak, Z.
Deposited on : 2021-10-28
Resolution : 2.55 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

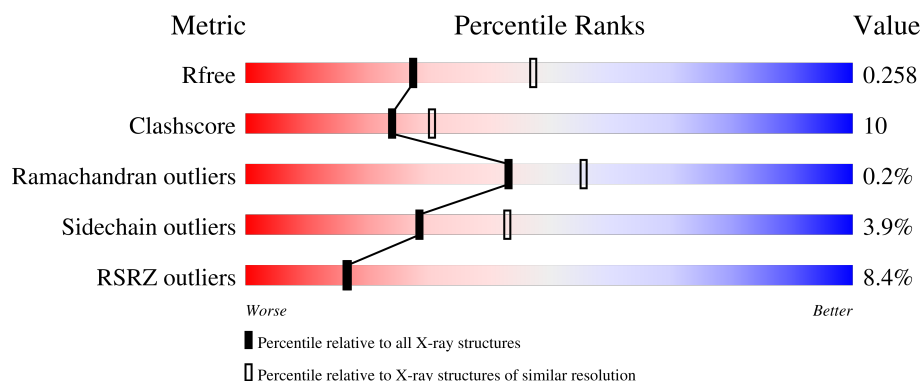
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	551	
1	B	551	
1	C	551	
1	D	551	

2 Entry composition [i](#)

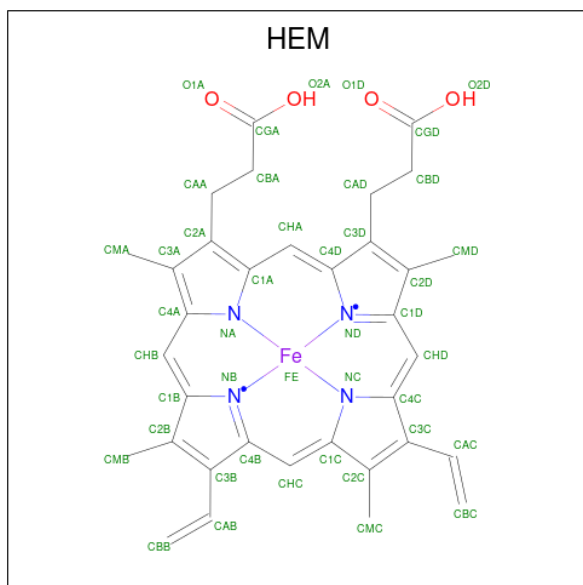
There are 4 unique types of molecules in this entry. The entry contains 14767 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3574	2278	638	635	23			
1	B	443	Total	C	N	O	S	0	0	0
			3568	2275	635	635	23			
1	C	440	Total	C	N	O	S	0	0	0
			3530	2253	624	630	23			
1	D	439	Total	C	N	O	S	0	0	0
			3458	2212	602	622	22			

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



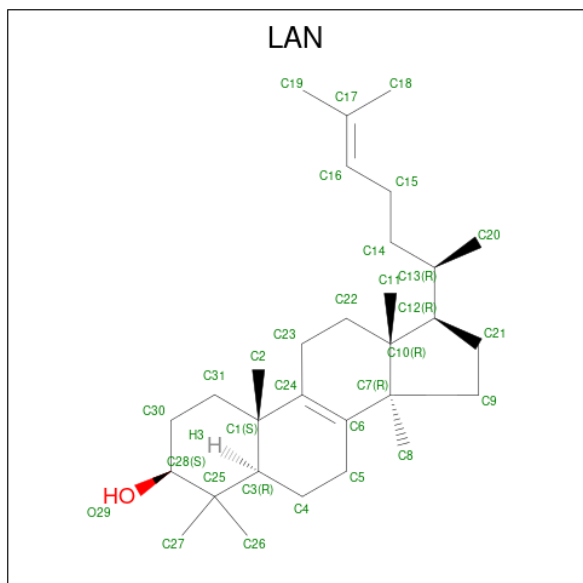
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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

- Molecule 3 is LANOSTEROL (CCD ID: LAN) (formula: $C_{30}H_{50}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			31 30 1			
3	B	1	Total	C O	0	0
			31 30 1			
3	C	1	Total	C O	0	0
			31 30 1			
3	D	1	Total	C O	0	0
			31 30 1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103 103			
4	B	95	Total	O	0	0
			95 95			
4	C	66	Total	O	0	0
			66 66			

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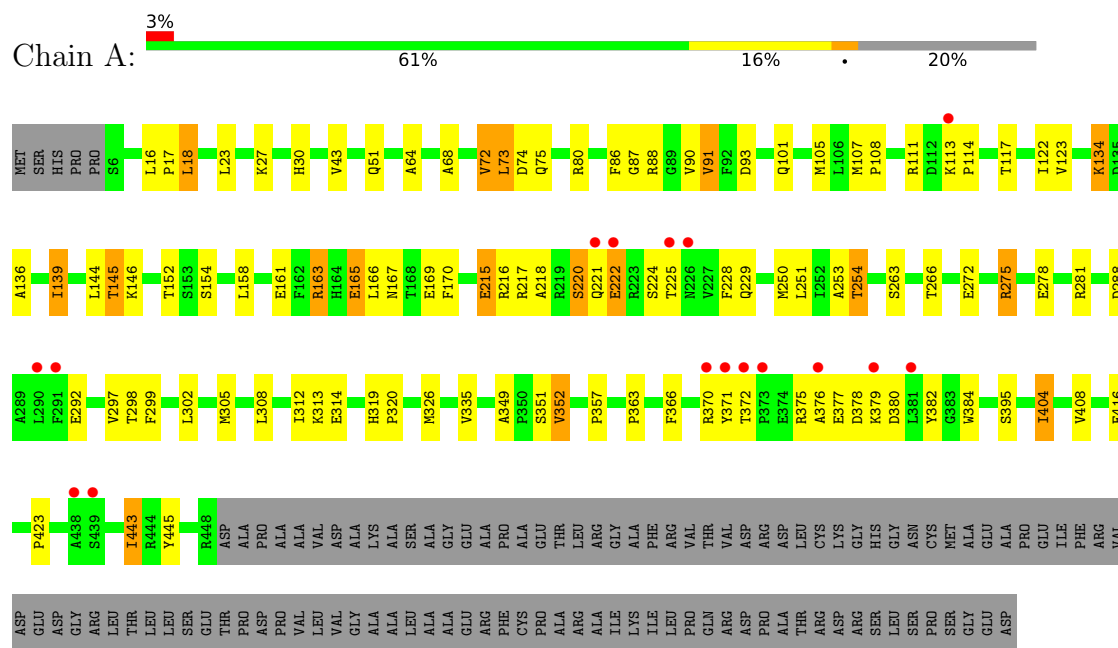
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	77	Total	O	0	0
			77	77		

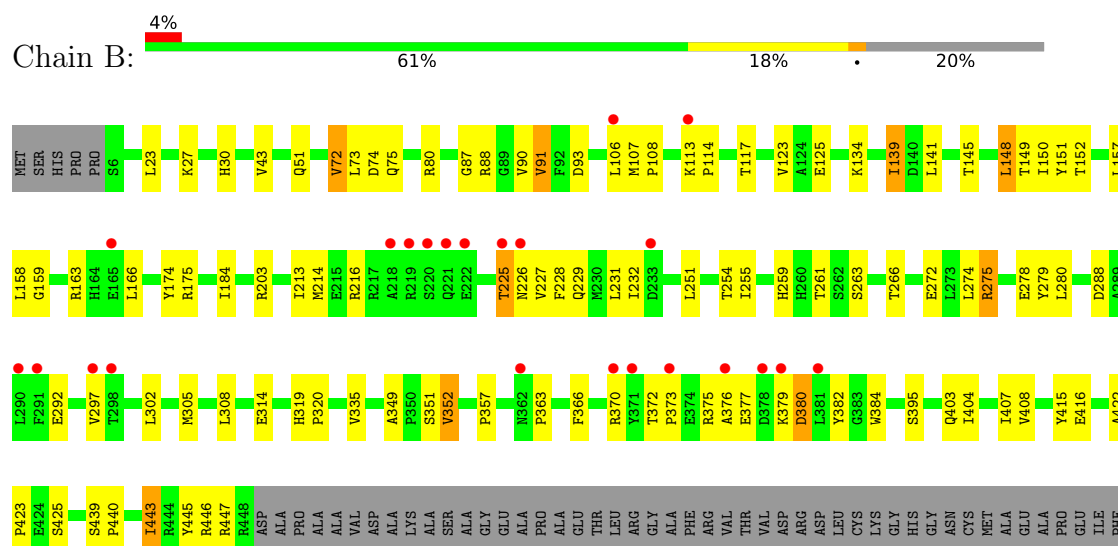
3 Residue-property plots

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: Cytochrome P450 51



• Molecule 1: Cytochrome P450 51



Chain C: 7% 59% 19% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.21Å 206.16Å 81.43Å 90.00° 114.09° 90.00°	Depositor
Resolution (Å)	74.45 – 2.55 74.45 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (74.45-2.55) 99.0 (74.45-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.246 0.208 , 0.258	Depositor DCC
R_{free} test set	3792 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14767	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: LAN, 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	0.96	0/3657	1.31	4/4944 (0.1%)
1	B	0.96	0/3651	1.32	6/4937 (0.1%)
1	C	0.95	0/3612	1.31	3/4887 (0.1%)
1	D	0.96	0/3539	1.31	2/4795 (0.0%)
All	All	0.96	0/14459	1.31	15/19563 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLU	N-CA-C	-7.55	101.96	112.45
1	C	438	ALA	O-C-N	6.37	130.21	122.75
1	A	87	GLY	CA-C-O	-6.18	118.20	122.22
1	B	225	THR	CB-CA-C	-5.97	99.15	111.22
1	B	159	GLY	CA-C-O	-5.62	118.41	122.45
1	C	87	GLY	CA-C-O	-5.61	118.57	122.22
1	A	18	LEU	N-CA-CB	-5.42	108.00	114.17
1	A	220	SER	N-CA-C	-5.39	105.30	111.07
1	D	19	LEU	N-CA-C	-5.35	107.41	114.31
1	B	87	GLY	CA-C-O	-5.30	118.78	122.22
1	B	225	THR	N-CA-C	-5.26	102.12	109.69
1	B	375	ARG	N-CA-C	5.21	118.51	111.17
1	C	159	GLY	CA-C-O	-5.18	118.72	122.45
1	D	159	GLY	CA-C-O	-5.13	118.47	122.52
1	B	228	PHE	N-CA-C	-5.03	105.27	111.40

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	3574	0	3584	85	0
1	B	3568	0	3573	75	0
1	C	3530	0	3514	74	0
1	D	3458	0	3396	49	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	31	0	50	2	0
3	B	31	0	50	5	0
3	C	31	0	50	4	0
3	D	31	0	50	3	0
4	A	103	0	0	1	0
4	B	95	0	0	0	0
4	C	66	0	0	0	0
4	D	77	0	0	0	0
All	All	14767	0	14387	288	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 10.

All (288) 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:117:THR:HG23	1:B:373:PRO:HB3	1.43	1.00
1:A:370:ARG:HH22	1:A:384:TRP:NE1	1.69	0.89
1:B:225:THR:HG22	1:B:226:ASN:H	1.43	0.82
1:A:117:THR:CG2	1:B:373:PRO:HB3	2.11	0.81
1:B:149:THR:HA	1:B:152:THR:HG22	1.68	0.75
1:A:370:ARG:HH22	1:A:384:TRP:CD1	2.05	0.74
1:B:370:ARG:HH22	1:B:384:TRP:NE1	1.85	0.74
1:A:371:TYR:HA	1:A:375:ARG:NH1	2.03	0.73
1:A:117:THR:HG23	1:B:373:PRO:CB	2.18	0.73
1:B:415:TYR:CE1	1:B:447:ARG:HG2	2.24	0.72
2:B:601:HEM:HMC2	2:B:601:HEM:HBC2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:THR:HA	1:B:152:THR:CG2	2.20	0.71
1:C:142:LEU:O	1:C:145:THR:HG22	1.91	0.70
1:C:145:THR:OG1	1:C:266:THR:HG23	1.91	0.70
1:B:376:ALA:HA	1:B:379:LYS:HD3	1.74	0.69
1:C:307:GLN:O	1:C:311:VAL:HG13	1.93	0.69
1:B:225:THR:O	1:B:229:GLN:HB2	1.94	0.68
1:A:145:THR:OG1	1:A:266:THR:HG23	1.93	0.67
1:D:257:ALA:HB2	3:D:602:LAN:H211	1.75	0.67
1:A:302:LEU:HD23	1:A:305:MET:HE2	1.77	0.66
1:A:370:ARG:HH21	1:A:377:GLU:HB3	1.60	0.66
1:A:272:GLU:HG2	1:A:366:PHE:CE2	2.31	0.66
1:B:152:THR:HG23	1:B:403:GLN:OE1	1.96	0.66
2:D:601:HEM:HBC2	2:D:601:HEM:HMC2	1.79	0.65
3:B:602:LAN:H2C3	3:B:602:LAN:H262	1.78	0.65
1:A:371:TYR:HA	1:A:375:ARG:HH12	1.61	0.65
1:C:416:GLU:O	1:C:445:TYR:HA	1.97	0.65
1:D:272:GLU:HG2	1:D:366:PHE:CE2	2.33	0.63
1:C:174:TYR:CZ	1:C:255:ILE:HD12	2.34	0.63
1:A:370:ARG:NH2	1:A:384:TRP:CD1	2.67	0.63
1:C:272:GLU:HG2	1:C:366:PHE:CE1	2.34	0.63
1:B:225:THR:HG22	1:B:226:ASN:N	2.13	0.63
1:D:125:GLU:OE2	1:D:163:ARG:NH2	2.31	0.63
2:A:601:HEM:HBC2	2:A:601:HEM:HMC2	1.80	0.63
1:B:251:LEU:O	1:B:254:THR:HG22	1.99	0.63
3:A:602:LAN:H262	3:A:602:LAN:H2C3	1.81	0.62
1:B:370:ARG:HH22	1:B:384:TRP:CD1	2.17	0.62
3:C:602:LAN:H262	3:C:602:LAN:H2C3	1.82	0.62
1:A:17:PRO:O	1:A:18:LEU:HB2	2.00	0.62
1:B:114:PRO:O	1:B:117:THR:HB	2.00	0.61
3:D:602:LAN:H2C3	3:D:602:LAN:H262	1.82	0.61
1:A:114:PRO:O	1:A:117:THR:HB	1.99	0.61
1:B:445:TYR:O	1:B:446:ARG:HG3	2.01	0.61
1:B:157:LEU:O	1:B:227:VAL:HG11	2.01	0.60
1:A:161:GLU:HB3	1:A:217:ARG:HH21	1.65	0.60
1:B:272:GLU:HG2	1:B:366:PHE:CE1	2.36	0.60
1:D:255:ILE:O	1:D:259:HIS:HB3	2.01	0.60
1:B:302:LEU:HD23	1:B:305:MET:HE2	1.83	0.59
1:C:349:ALA:HB1	1:C:352:VAL:HG13	1.85	0.59
1:B:370:ARG:HH21	1:B:377:GLU:HB3	1.68	0.58
1:D:124:ALA:O	1:D:128:ALA:N	2.37	0.58
1:A:349:ALA:HB1	1:A:352:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:MET:HE1	4:A:728:HOH:O	2.03	0.58
1:B:158:LEU:HD21	1:B:254:THR:HG21	1.84	0.58
1:C:210:VAL:O	1:C:214:MET:HG3	2.04	0.58
1:D:439:SER:HB3	1:D:440:PRO:HD3	1.86	0.58
1:A:225:THR:OG1	1:D:39:GLU:HG3	2.04	0.57
1:B:349:ALA:HB1	1:B:352:VAL:HG13	1.86	0.57
1:B:90:VAL:HG12	1:B:91:VAL:HG23	1.87	0.57
1:A:154:SER:CB	1:A:166:LEU:HD11	2.35	0.57
1:B:148:LEU:O	1:B:152:THR:HG22	2.04	0.57
1:B:227:VAL:O	1:B:231:LEU:HG	2.05	0.57
1:B:372:THR:HB	1:B:373:PRO:HD2	1.85	0.57
1:D:155:HIS:CE1	1:D:160:ALA:HB2	2.41	0.56
1:C:269:VAL:HG21	1:C:312:ILE:HG22	1.87	0.56
1:A:122:ILE:HG12	1:A:152:THR:HG23	1.88	0.56
1:B:107:MET:N	1:B:108:PRO:HD2	2.21	0.56
1:C:268:TRP:CE2	1:C:437:PRO:HG3	2.39	0.56
1:C:130:LEU:HD11	1:C:411:LEU:HD23	1.88	0.56
1:C:302:LEU:HD12	1:C:402:PHE:CE1	2.40	0.56
1:D:417:PHE:HA	1:D:444:ARG:O	2.05	0.56
1:B:72:VAL:HG23	1:B:73:LEU:HD13	1.88	0.55
1:A:218:ALA:O	1:A:221:GLN:HB2	2.07	0.55
1:C:439:SER:HB2	1:C:440:PRO:HD3	1.88	0.55
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.36	0.55
1:C:227:VAL:O	1:C:230:MET:HB3	2.06	0.55
1:B:149:THR:CA	1:B:152:THR:HG22	2.37	0.55
1:A:375:ARG:NH1	1:A:377:GLU:OE2	2.40	0.54
1:B:213:ILE:HG12	1:B:216:ARG:HH22	1.72	0.54
1:A:224:SER:HA	1:A:229:GLN:HG3	1.89	0.54
1:C:268:TRP:NE1	1:C:437:PRO:HG3	2.22	0.54
1:A:107:MET:N	1:A:108:PRO:HD2	2.23	0.54
1:B:214:MET:HG2	1:B:232:ILE:HG12	1.89	0.54
1:B:278:GLU:HG2	1:B:279:TYR:N	2.22	0.54
1:D:221:GLN:O	1:D:222:GLU:C	2.51	0.54
1:C:142:LEU:HD12	1:C:145:THR:HG21	1.90	0.53
2:D:601:HEM:HBC2	2:D:601:HEM:CMC	2.38	0.53
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.38	0.53
1:B:372:THR:HB	1:B:373:PRO:CD	2.39	0.53
1:C:107:MET:N	1:C:108:PRO:HD2	2.24	0.52
1:D:111:ARG:O	1:D:114:PRO:HD2	2.09	0.52
1:D:406:ALA:HA	1:D:409:CYS:SG	2.49	0.52
1:C:30:HIS:CD2	1:C:351:SER:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:HD12	1:C:145:THR:CG2	2.39	0.52
1:C:82:MET:HE3	3:C:602:LAN:H263	1.90	0.52
1:C:370:ARG:C	1:C:372:THR:H	2.17	0.52
1:A:101:GLN:O	1:A:105:MET:HG3	2.10	0.52
1:C:288:ASP:O	1:C:292:GLU:HG2	2.11	0.51
1:B:370:ARG:NH2	1:B:384:TRP:CD1	2.78	0.51
1:A:161:GLU:HB3	1:A:217:ARG:NH2	2.25	0.51
1:C:136:ALA:HB2	1:C:446:ARG:HG2	1.92	0.51
1:D:113:LYS:HB2	1:D:114:PRO:HD3	1.93	0.51
1:B:113:LYS:HB2	1:B:114:PRO:HD3	1.93	0.50
1:A:90:VAL:HG12	1:A:91:VAL:HG23	1.92	0.50
1:A:416:GLU:O	1:A:445:TYR:HA	2.11	0.50
1:A:113:LYS:HB2	1:A:114:PRO:HD3	1.93	0.50
1:B:415:TYR:CZ	1:B:447:ARG:HG2	2.45	0.50
1:C:152:THR:HG22	1:C:403:GLN:OE1	2.12	0.50
1:A:145:THR:HG21	1:A:263:SER:O	2.11	0.50
1:C:123:VAL:HG21	1:C:297:VAL:CG2	2.42	0.49
1:A:111:ARG:O	1:A:114:PRO:HD2	2.12	0.49
1:B:30:HIS:CD2	1:B:351:SER:HB2	2.46	0.49
1:D:119:SER:O	1:D:123:VAL:HG23	2.12	0.49
1:B:23:LEU:O	1:B:27:LYS:HG2	2.12	0.49
1:A:30:HIS:CD2	1:A:351:SER:HB2	2.47	0.49
1:A:225:THR:HG22	1:A:225:THR:O	2.13	0.49
1:B:106:LEU:HB2	3:B:602:LAN:H192	1.94	0.49
1:C:23:LEU:O	1:C:27:LYS:HG2	2.13	0.49
1:D:257:ALA:O	1:D:261:THR:OG1	2.27	0.49
1:C:103:LEU:HD23	3:C:602:LAN:H183	1.94	0.49
1:A:23:LEU:O	1:A:27:LYS:HG2	2.13	0.48
1:C:101:GLN:O	1:C:105:MET:HG3	2.12	0.48
1:A:298:THR:HG22	1:A:299:PHE:H	1.77	0.48
1:B:416:GLU:O	1:B:445:TYR:HA	2.13	0.48
1:A:220:SER:C	1:A:222:GLU:H	2.22	0.48
1:A:72:VAL:HG23	1:A:73:LEU:HD13	1.95	0.48
1:B:107:MET:HE1	1:B:395:SER:OG	2.13	0.48
1:D:439:SER:HB3	1:D:440:PRO:CD	2.43	0.48
1:C:122:ILE:HG12	1:C:152:THR:HG23	1.94	0.48
1:C:445:TYR:O	1:C:446:ARG:HG3	2.14	0.48
1:A:220:SER:C	1:A:222:GLU:N	2.71	0.48
1:A:250:MET:O	1:A:254:THR:HB	2.14	0.47
1:B:275:ARG:HD2	1:B:423:PRO:O	2.14	0.47
1:C:113:LYS:CB	1:C:114:PRO:HD3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:GLU:HG2	1:D:378:ASP:N	2.28	0.47
1:A:117:THR:CB	1:B:373:PRO:HB3	2.45	0.47
1:C:126:VAL:HG22	1:C:148:LEU:HD11	1.96	0.47
1:D:284:ARG:HD3	1:D:448:ARG:NH1	2.28	0.47
1:C:377:GLU:HG2	1:C:378:ASP:N	2.29	0.47
1:C:255:ILE:O	1:C:259:HIS:HB3	2.15	0.47
1:A:275:ARG:HD2	1:A:423:PRO:O	2.15	0.47
1:B:174:TYR:OH	1:B:255:ILE:HD12	2.15	0.47
1:C:291:PHE:CG	1:C:413:ARG:HD3	2.50	0.47
1:A:51:GLN:HE22	1:A:80:ARG:HH22	1.63	0.47
1:A:377:GLU:HG2	1:A:378:ASP:N	2.30	0.47
1:C:141:LEU:O	1:C:145:THR:HB	2.15	0.47
1:D:82:MET:HE3	3:D:602:LAN:H263	1.96	0.47
1:C:51:GLN:OE1	1:C:53:MET:CE	2.63	0.46
1:C:370:ARG:C	1:C:372:THR:N	2.74	0.46
1:C:420:ALA:HA	1:C:444:ARG:NH1	2.31	0.46
1:A:139:ILE:HG13	1:A:443:ILE:HG22	1.96	0.46
1:C:206:LEU:O	1:C:210:VAL:HG23	2.16	0.46
1:A:123:VAL:HG21	1:A:297:VAL:CG1	2.45	0.46
1:B:380:ASP:C	1:B:382:TYR:H	2.23	0.46
1:D:312:ILE:HG21	1:D:404:ILE:HD11	1.96	0.46
1:C:97:GLU:CD	1:C:97:GLU:H	2.24	0.46
1:C:269:VAL:CG2	1:C:312:ILE:HG22	2.46	0.46
1:A:107:MET:HE1	1:A:395:SER:OG	2.15	0.46
1:C:56:LEU:HG	1:C:346:VAL:HG23	1.98	0.46
1:C:63:GLU:HG3	1:C:67:ARG:HD3	1.98	0.46
1:D:218:ALA:O	1:D:219:ARG:C	2.58	0.46
1:B:88:ARG:HA	1:B:93:ASP:OD2	2.16	0.45
1:A:68:ALA:CB	1:A:73:LEU:HD22	2.46	0.45
1:A:217:ARG:HH12	1:A:228:PHE:HE2	1.62	0.45
1:B:254:THR:HB	3:B:602:LAN:H193	1.98	0.45
1:D:270:LEU:CD1	1:D:412:LEU:HD21	2.46	0.45
1:B:439:SER:HB2	1:B:440:PRO:HD3	1.98	0.45
1:D:406:ALA:O	1:D:410:VAL:HG23	2.16	0.45
1:B:272:GLU:HG2	1:B:366:PHE:CD1	2.51	0.45
1:C:175:ARG:HD2	1:C:175:ARG:HA	1.67	0.45
1:A:375:ARG:HD3	1:A:377:GLU:OE2	2.16	0.45
1:B:123:VAL:HG21	1:B:297:VAL:CG1	2.47	0.45
1:C:217:ARG:NH1	1:C:228:PHE:HE2	2.14	0.45
1:B:404:ILE:O	1:B:408:VAL:HG13	2.16	0.45
1:B:74:ASP:OD1	1:B:75:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:THR:OG1	3:A:602:LAN:C19	2.66	0.44
1:A:88:ARG:HA	1:A:93:ASP:OD2	2.16	0.44
1:C:88:ARG:HA	1:C:93:ASP:OD2	2.17	0.44
1:A:217:ARG:NH1	1:A:228:PHE:CE2	2.85	0.44
1:C:257:ALA:HB1	2:C:601:HEM:C3C	2.52	0.44
1:D:88:ARG:HA	1:D:93:ASP:OD2	2.18	0.44
1:C:139:ILE:HG13	1:C:443:ILE:HG22	2.00	0.44
1:D:125:GLU:CD	1:D:163:ARG:NH2	2.75	0.44
1:A:163:ARG:HD2	1:A:166:LEU:HD12	1.99	0.44
1:A:370:ARG:C	1:A:372:THR:H	2.25	0.44
1:B:308:LEU:HD11	1:B:408:VAL:HG21	1.99	0.44
1:C:123:VAL:CG2	1:C:297:VAL:CG2	2.95	0.44
1:B:125:GLU:OE2	1:B:163:ARG:NH2	2.51	0.44
1:B:152:THR:HG21	1:B:407:ILE:HD11	1.98	0.44
1:C:62:SER:O	1:C:66:TYR:CD2	2.71	0.44
1:A:380:ASP:C	1:A:382:TYR:H	2.25	0.43
1:C:51:GLN:HE22	1:C:80:ARG:HH22	1.65	0.43
1:C:308:LEU:O	1:C:311:VAL:HG22	2.18	0.43
1:B:51:GLN:HE22	1:B:80:ARG:HH22	1.67	0.43
1:D:278:GLU:HG2	1:D:279:TYR:N	2.33	0.43
1:A:312:ILE:HG21	1:A:404:ILE:HD11	1.99	0.43
2:B:601:HEM:C3D	3:B:602:LAN:H203	2.53	0.43
1:C:380:ASP:C	1:C:382:TYR:H	2.26	0.43
1:B:357:PRO:HA	1:B:363:PRO:HG3	2.00	0.43
1:A:117:THR:OG1	1:B:373:PRO:HB3	2.18	0.43
1:A:404:ILE:O	1:A:408:VAL:HG13	2.19	0.43
1:D:118:TYR:CE1	1:D:156:CYS:O	2.71	0.43
1:D:125:GLU:CD	1:D:163:ARG:HH21	2.27	0.43
1:D:278:GLU:HG2	1:D:279:TYR:CD2	2.54	0.43
1:B:254:THR:CB	3:B:602:LAN:H193	2.48	0.43
1:C:228:PHE:HE1	1:C:251:LEU:HD11	1.83	0.43
1:A:380:ASP:C	1:A:382:TYR:N	2.77	0.43
1:D:126:VAL:HG22	1:D:148:LEU:HD21	2.00	0.43
1:D:218:ALA:C	1:D:220:SER:N	2.76	0.43
1:A:308:LEU:HD11	1:A:408:VAL:HG21	2.01	0.43
1:A:376:ALA:HA	1:A:379:LYS:HE2	2.01	0.43
1:D:134:LYS:O	1:D:136:ALA:N	2.46	0.43
1:B:139:ILE:HG13	1:B:443:ILE:HG22	2.01	0.42
1:C:251:LEU:O	1:C:255:ILE:HG13	2.19	0.42
1:C:314:GLU:OE1	1:C:314:GLU:HA	2.19	0.42
1:A:146:LYS:HA	1:A:263:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:HD23	1:B:280:LEU:HD22	2.01	0.42
1:C:217:ARG:NH1	1:C:228:PHE:CE2	2.87	0.42
1:C:323:ILE:HD13	1:C:435:VAL:CG2	2.49	0.42
1:D:206:LEU:HD23	1:D:252:ILE:CG1	2.49	0.42
1:A:74:ASP:OD1	1:A:75:GLN:N	2.52	0.42
1:C:134:LYS:O	1:C:136:ALA:N	2.52	0.42
1:A:167:ASN:H	1:A:170:PHE:HB2	1.85	0.42
1:D:144:LEU:HD13	1:D:144:LEU:HA	1.96	0.42
1:A:288:ASP:O	1:A:292:GLU:HG2	2.19	0.42
1:B:255:ILE:O	1:B:259:HIS:HB3	2.20	0.42
1:B:288:ASP:O	1:B:292:GLU:HG2	2.20	0.42
1:B:380:ASP:C	1:B:382:TYR:N	2.76	0.42
1:D:380:ASP:C	1:D:382:TYR:H	2.27	0.42
1:A:220:SER:HB2	1:A:222:GLU:HG2	2.00	0.42
1:B:150:ILE:HG22	1:B:166:LEU:HD21	2.01	0.42
1:D:106:LEU:C	1:D:108:PRO:HD2	2.44	0.42
1:D:158:LEU:HD21	1:D:254:THR:HG21	2.01	0.42
1:A:319:HIS:N	1:A:320:PRO:CD	2.83	0.42
1:B:263:SER:O	1:B:266:THR:HG22	2.18	0.42
1:C:230:MET:HB3	1:C:230:MET:HE3	1.86	0.42
1:C:323:ILE:HG21	1:C:435:VAL:HG21	2.02	0.42
1:A:376:ALA:HA	1:A:379:LYS:HD3	2.02	0.42
1:C:65:PHE:CD1	1:C:346:VAL:HG22	2.55	0.42
1:A:43:VAL:HG21	1:A:335:VAL:HG23	2.02	0.42
1:C:217:ARG:HH12	1:C:228:PHE:HE2	1.67	0.42
1:A:165:GLU:OE2	1:A:216:ARG:NH2	2.52	0.41
1:C:130:LEU:O	1:C:133:TRP:HB2	2.19	0.41
1:A:16:LEU:HD12	1:A:23:LEU:HD12	2.02	0.41
1:C:121:ILE:HG23	1:C:155:HIS:CG	2.55	0.41
1:A:272:GLU:HG2	1:A:366:PHE:CD2	2.55	0.41
1:B:151:TYR:CD1	1:B:166:LEU:HD23	2.55	0.41
1:C:82:MET:HE3	3:C:602:LAN:C26	2.50	0.41
1:D:63:GLU:HG2	1:D:67:ARG:HD3	2.02	0.41
1:B:175:ARG:HD2	1:B:175:ARG:HA	1.65	0.41
1:C:380:ASP:C	1:C:382:TYR:N	2.77	0.41
1:C:439:SER:HB2	1:C:440:PRO:CD	2.49	0.41
1:D:139:ILE:HG13	1:D:443:ILE:HG22	2.01	0.41
1:A:134:LYS:O	1:A:136:ALA:N	2.54	0.41
1:A:314:GLU:OE1	1:A:314:GLU:HA	2.21	0.41
1:B:123:VAL:CG2	1:B:297:VAL:CG1	2.98	0.41
1:D:275:ARG:HG3	1:D:419:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:GLU:HA	1:D:314:GLU:OE1	2.20	0.41
1:A:221:GLN:O	1:A:221:GLN:HG3	2.21	0.41
1:B:43:VAL:HG21	1:B:335:VAL:HG23	2.02	0.41
1:D:104:GLN:O	1:D:108:PRO:HD3	2.21	0.41
1:A:86:PHE:CE1	1:A:253:ALA:HA	2.56	0.41
1:A:263:SER:O	1:A:266:THR:HG22	2.20	0.41
1:B:422:ALA:O	1:B:425:SER:HB3	2.21	0.41
1:B:314:GLU:OE1	1:B:314:GLU:HA	2.20	0.41
1:A:123:VAL:CG2	1:A:297:VAL:CG1	2.99	0.41
1:A:145:THR:CG2	1:A:263:SER:O	2.68	0.41
1:A:215:GLU:HA	1:A:215:GLU:OE2	2.20	0.41
1:B:141:LEU:O	1:B:145:THR:HG23	2.21	0.41
1:C:357:PRO:HA	1:C:363:PRO:HG3	2.02	0.41
1:D:107:MET:N	1:D:108:PRO:HD2	2.36	0.41
1:D:380:ASP:C	1:D:382:TYR:N	2.79	0.41
1:A:27:LYS:HA	1:A:27:LYS:HD3	1.88	0.41
1:A:158:LEU:HD13	1:A:251:LEU:HD22	2.02	0.41
1:C:319:HIS:N	1:C:320:PRO:CD	2.84	0.41
1:D:107:MET:HB2	1:D:108:PRO:HD3	2.01	0.41
1:D:302:LEU:C	1:D:304:GLN:H	2.29	0.41
1:A:64:ALA:CB	1:A:335:VAL:HG12	2.51	0.40
1:B:319:HIS:N	1:B:320:PRO:CD	2.84	0.40
1:D:158:LEU:HD22	1:D:251:LEU:HD23	2.03	0.40
1:A:357:PRO:HA	1:A:363:PRO:HG3	2.03	0.40
1:C:51:GLN:HB3	1:C:53:MET:CE	2.52	0.40
1:D:68:ALA:CB	1:D:73:LEU:HD22	2.52	0.40
1:D:272:GLU:HG2	1:D:366:PHE:CD2	2.55	0.40
1:A:278:GLU:HA	1:A:281:ARG:HD3	2.04	0.40
1:C:64:ALA:CB	1:C:335:VAL:HG12	2.52	0.40
1:B:261:THR:HB	2:B:601:HEM:C3B	2.57	0.40
1:C:275:ARG:HD2	1:C:423:PRO:O	2.21	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	441/551 (80%)	412 (93%)	28 (6%)	1 (0%)	43	56
1	B	441/551 (80%)	415 (94%)	25 (6%)	1 (0%)	43	56
1	C	436/551 (79%)	409 (94%)	26 (6%)	1 (0%)	43	56
1	D	435/551 (79%)	412 (95%)	22 (5%)	1 (0%)	43	56
All	All	1753/2204 (80%)	1648 (94%)	101 (6%)	4 (0%)	43	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	B	91	VAL
1	C	91	VAL
1	D	91	VAL

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	381/466 (82%)	365 (96%)	16 (4%)	26	40
1	B	380/466 (82%)	370 (97%)	10 (3%)	40	59
1	C	374/466 (80%)	354 (95%)	20 (5%)	20	31
1	D	360/466 (77%)	348 (97%)	12 (3%)	33	50
All	All	1495/1864 (80%)	1437 (96%)	58 (4%)	28	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	A	73	LEU
1	A	134	LYS
1	A	139	ILE

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Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	THR
1	A	163	ARG
1	A	165	GLU
1	A	169	GLU
1	A	215	GLU
1	A	254	THR
1	A	275	ARG
1	A	313	LYS
1	A	352	VAL
1	A	404	ILE
1	A	443	ILE
1	B	72	VAL
1	B	134	LYS
1	B	139	ILE
1	B	148	LEU
1	B	184	ILE
1	B	203	ARG
1	B	275	ARG
1	B	352	VAL
1	B	380	ASP
1	B	443	ILE
1	C	72	VAL
1	C	73	LEU
1	C	119	SER
1	C	134	LYS
1	C	139	ILE
1	C	144	LEU
1	C	145	THR
1	C	148	LEU
1	C	163	ARG
1	C	167	ASN
1	C	169	GLU
1	C	215	GLU
1	C	254	THR
1	C	255	ILE
1	C	275	ARG
1	C	311	VAL
1	C	346	VAL
1	C	352	VAL
1	C	404	ILE
1	C	443	ILE

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Mol	Chain	Res	Type
1	D	139	ILE
1	D	144	LEU
1	D	163	ARG
1	D	169	GLU
1	D	221	GLN
1	D	254	THR
1	D	273	LEU
1	D	305	MET
1	D	355	ARG
1	D	373	PRO
1	D	404	ILE
1	D	443	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	229	GLN
1	B	30	HIS
1	B	75	GLN
1	B	221	GLN
1	C	30	HIS
1	C	164	HIS
1	D	336	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	C	601	1	50,50,50	1.58	8 (16%)	67,82,82	1.75	15 (22%)
2	HEM	A	601	1	50,50,50	1.58	8 (16%)	67,82,82	1.68	13 (19%)
2	HEM	D	601	1	50,50,50	1.59	8 (16%)	67,82,82	1.76	14 (20%)
3	LAN	C	602	-	34,34,34	0.40	0	56,56,56	0.64	0
3	LAN	A	602	-	34,34,34	0.39	0	56,56,56	0.67	0
3	LAN	D	602	-	34,34,34	0.39	0	56,56,56	0.64	0
3	LAN	B	602	-	34,34,34	0.40	0	56,56,56	0.63	1 (1%)
2	HEM	B	601	1	50,50,50	1.57	8 (16%)	67,82,82	1.72	17 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	601	1	-	3/14/54/54	-
2	HEM	A	601	1	-	3/14/54/54	-
2	HEM	D	601	1	-	1/14/54/54	-
3	LAN	C	602	-	-	0/10/82/82	0/4/4/4
3	LAN	A	602	-	-	3/10/82/82	0/4/4/4
3	LAN	D	602	-	-	0/10/82/82	0/4/4/4
3	LAN	B	602	-	-	1/10/82/82	0/4/4/4
2	HEM	B	601	1	-	2/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	FE-NB	5.10	2.10	1.94
2	A	601	HEM	FE-NB	5.05	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	FE-NB	5.01	2.10	1.94
2	C	601	HEM	FE-NB	5.00	2.10	1.94
2	C	601	HEM	FE-NC	4.26	2.09	1.95
2	B	601	HEM	FE-NC	4.22	2.09	1.95
2	A	601	HEM	FE-NC	4.21	2.09	1.95
2	D	601	HEM	FE-NC	4.20	2.09	1.95
2	D	601	HEM	C1B-NB	-3.53	1.34	1.40
2	C	601	HEM	C1B-NB	-3.52	1.34	1.40
2	A	601	HEM	C1B-NB	-3.51	1.34	1.40
2	B	601	HEM	C1B-NB	-3.49	1.34	1.40
2	D	601	HEM	C4D-ND	-3.41	1.34	1.40
2	C	601	HEM	C4D-ND	-3.37	1.34	1.40
2	A	601	HEM	C4D-ND	-3.37	1.34	1.40
2	B	601	HEM	C4D-ND	-3.35	1.34	1.40
2	D	601	HEM	FE-ND	-2.95	1.85	1.94
2	C	601	HEM	FE-ND	-2.86	1.86	1.94
2	B	601	HEM	FE-ND	-2.83	1.86	1.94
2	A	601	HEM	FE-ND	-2.80	1.86	1.94
2	D	601	HEM	C1D-ND	-2.43	1.34	1.38
2	A	601	HEM	C1D-ND	-2.40	1.34	1.38
2	B	601	HEM	C1D-ND	-2.34	1.34	1.38
2	C	601	HEM	C1D-ND	-2.34	1.34	1.38
2	D	601	HEM	C1C-C2C	-2.31	1.40	1.45
2	C	601	HEM	C1C-C2C	-2.29	1.40	1.45
2	C	601	HEM	C4B-NB	-2.29	1.34	1.38
2	A	601	HEM	C4B-NB	-2.29	1.34	1.38
2	D	601	HEM	C4B-NB	-2.28	1.34	1.38
2	B	601	HEM	C4B-NB	-2.26	1.34	1.38
2	A	601	HEM	C1C-C2C	-2.23	1.40	1.45
2	B	601	HEM	C1C-C2C	-2.23	1.40	1.45

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	CHC-C4B-NB	5.88	130.75	124.42
2	D	601	HEM	CHC-C4B-NB	5.43	130.27	124.42
2	C	601	HEM	CHC-C4B-NB	5.37	130.20	124.42
2	A	601	HEM	CHC-C4B-NB	5.27	130.09	124.42
2	D	601	HEM	CHD-C1D-ND	5.15	129.97	124.42
2	B	601	HEM	CHD-C1D-ND	4.97	129.77	124.42
2	C	601	HEM	CHD-C1D-ND	4.73	129.52	124.42
2	A	601	HEM	CHD-C1D-ND	4.53	129.30	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	CHB-C1B-NB	4.05	129.37	124.37
2	C	601	HEM	CHA-C4D-ND	3.99	129.31	124.37
2	D	601	HEM	CHB-C1B-NB	3.84	129.12	124.37
2	D	601	HEM	CHD-C1D-C2D	-3.67	119.23	125.03
2	B	601	HEM	CHD-C1D-C2D	-3.67	119.24	125.03
2	A	601	HEM	CHB-C1B-NB	3.65	128.89	124.37
2	D	601	HEM	CHA-C4D-ND	3.64	128.87	124.37
2	A	601	HEM	CHD-C1D-C2D	-3.57	119.39	125.03
2	C	601	HEM	CHD-C1D-C2D	-3.47	119.54	125.03
2	B	601	HEM	CHA-C4D-ND	3.26	128.40	124.37
2	A	601	HEM	CHA-C4D-ND	3.17	128.28	124.37
2	B	601	HEM	CHB-C1B-NB	3.08	128.17	124.37
2	D	601	HEM	CHA-C4D-C3D	-3.00	119.70	125.23
2	C	601	HEM	CHA-C4D-C3D	-2.94	119.81	125.23
2	A	601	HEM	CHA-C4D-C3D	-2.90	119.87	125.23
2	D	601	HEM	C1B-NB-C4B	2.81	108.53	105.21
2	C	601	HEM	C1B-NB-C4B	2.76	108.47	105.21
2	B	601	HEM	CHA-C4D-C3D	-2.72	120.20	125.23
2	A	601	HEM	C1B-NB-C4B	2.71	108.42	105.21
2	C	601	HEM	CHB-C1B-C2B	-2.63	119.47	126.95
2	D	601	HEM	C1A-CHA-C4D	-2.56	120.22	126.25
2	C	601	HEM	C1A-CHA-C4D	-2.54	120.26	126.25
2	B	601	HEM	C1B-NB-C4B	2.53	108.20	105.21
2	A	601	HEM	O2D-CGD-CBD	2.51	121.94	114.00
2	D	601	HEM	CAD-C3D-C4D	2.50	129.05	124.70
2	B	601	HEM	CAD-C3D-C4D	2.49	129.04	124.70
2	D	601	HEM	CHB-C1B-C2B	-2.44	120.02	126.95
2	A	601	HEM	CHB-C1B-C2B	-2.39	120.15	126.95
2	A	601	HEM	C1A-CHA-C4D	-2.39	120.64	126.25
2	B	601	HEM	CHC-C4B-C3B	-2.37	120.34	125.07
2	C	601	HEM	CAD-CBD-CGD	-2.34	107.45	113.67
2	B	601	HEM	O2D-CGD-CBD	2.29	121.24	114.00
2	B	601	HEM	C4B-C3B-C2B	-2.27	105.19	107.28
2	A	601	HEM	CAD-C3D-C4D	2.27	128.65	124.70
2	B	601	HEM	C1A-CHA-C4D	-2.23	121.01	126.25
2	D	601	HEM	CHD-C4C-NC	2.22	126.88	124.45
2	D	601	HEM	CAD-CBD-CGD	-2.22	107.77	113.67
2	C	601	HEM	C4A-CHB-C1B	-2.19	121.10	126.25
2	D	601	HEM	C4C-CHD-C1D	-2.17	121.40	126.02
2	B	601	HEM	O2A-CGA-CBA	2.14	120.75	114.00
2	A	601	HEM	CAA-CBA-CGA	-2.12	108.03	113.67
2	B	601	HEM	C4C-CHD-C1D	-2.09	121.58	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	CHD-C4C-NC	2.09	126.73	124.45
2	B	601	HEM	CHB-C1B-C2B	-2.08	121.04	126.95
2	D	601	HEM	C4A-CHB-C1B	-2.08	121.36	126.25
2	C	601	HEM	O2D-CGD-CBD	2.06	120.52	114.00
2	C	601	HEM	C4C-CHD-C1D	-2.05	121.67	126.02
2	A	601	HEM	CHD-C4C-NC	2.02	126.65	124.45
2	B	601	HEM	O2A-CGA-O1A	-2.01	118.15	123.33
2	B	601	HEM	CHD-C4C-NC	2.01	126.64	124.45
3	B	602	LAN	C31-C1-C3	-2.01	106.14	108.36
2	C	601	HEM	C3B-C4B-NB	-2.01	108.03	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

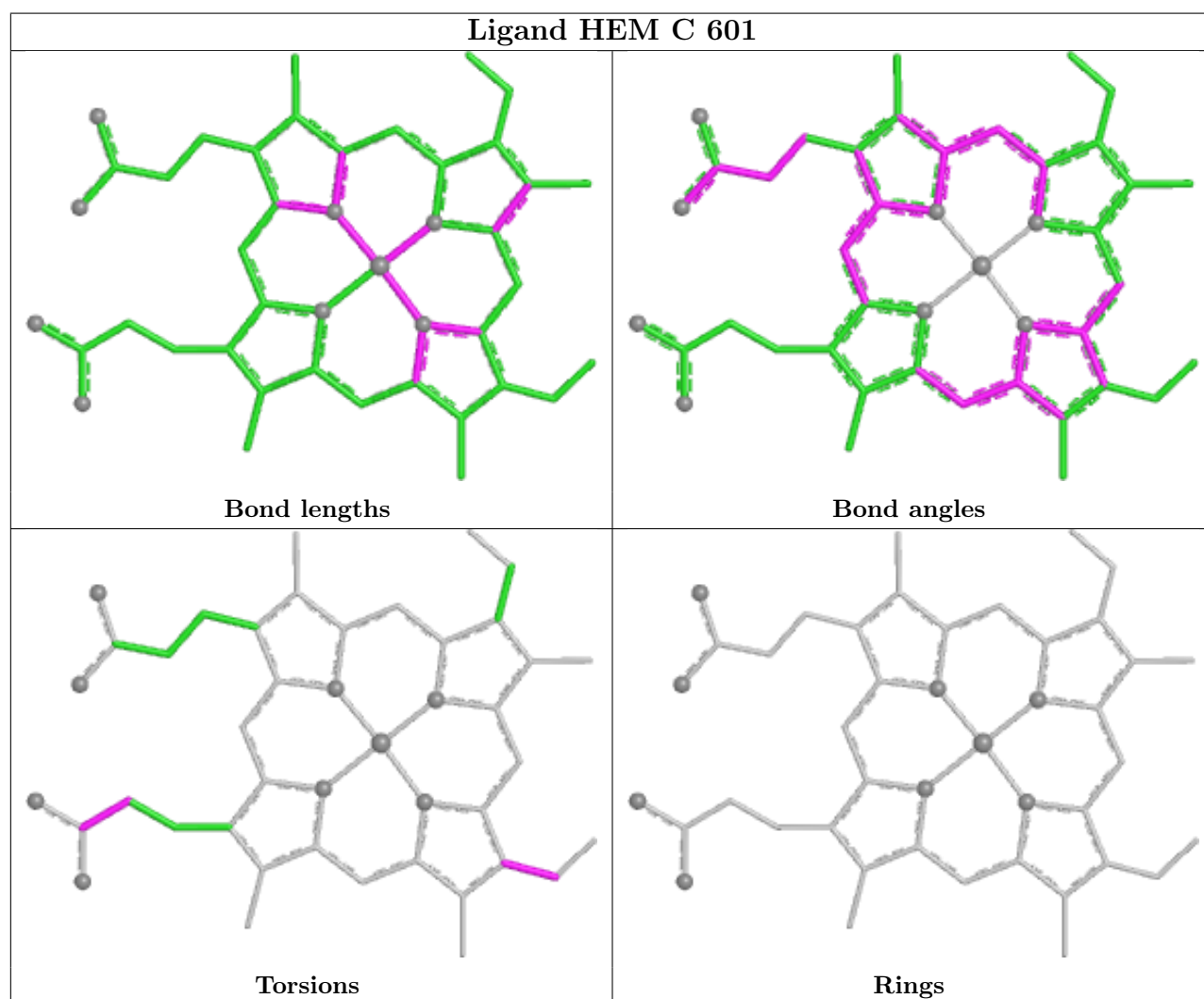
Mol	Chain	Res	Type	Atoms
3	A	602	LAN	C15-C16-C17-C19
3	A	602	LAN	C15-C16-C17-C18
3	B	602	LAN	C20-C13-C14-C15
3	A	602	LAN	C20-C13-C14-C15
2	B	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAD-CBD-CGD-O1D
2	C	601	HEM	C2B-C3B-CAB-CBB
2	A	601	HEM	CAA-CBA-CGA-O2A

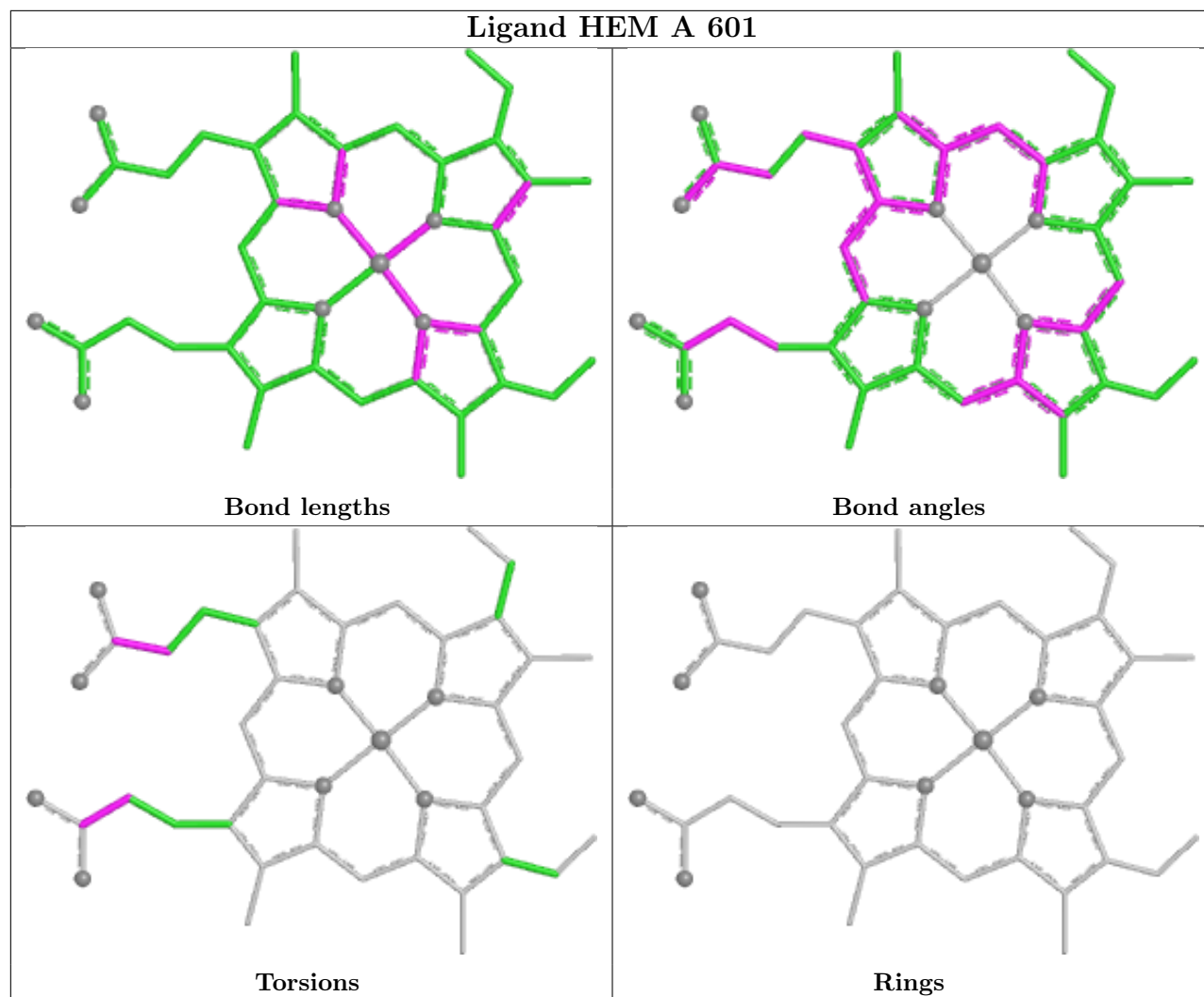
There are no ring outliers.

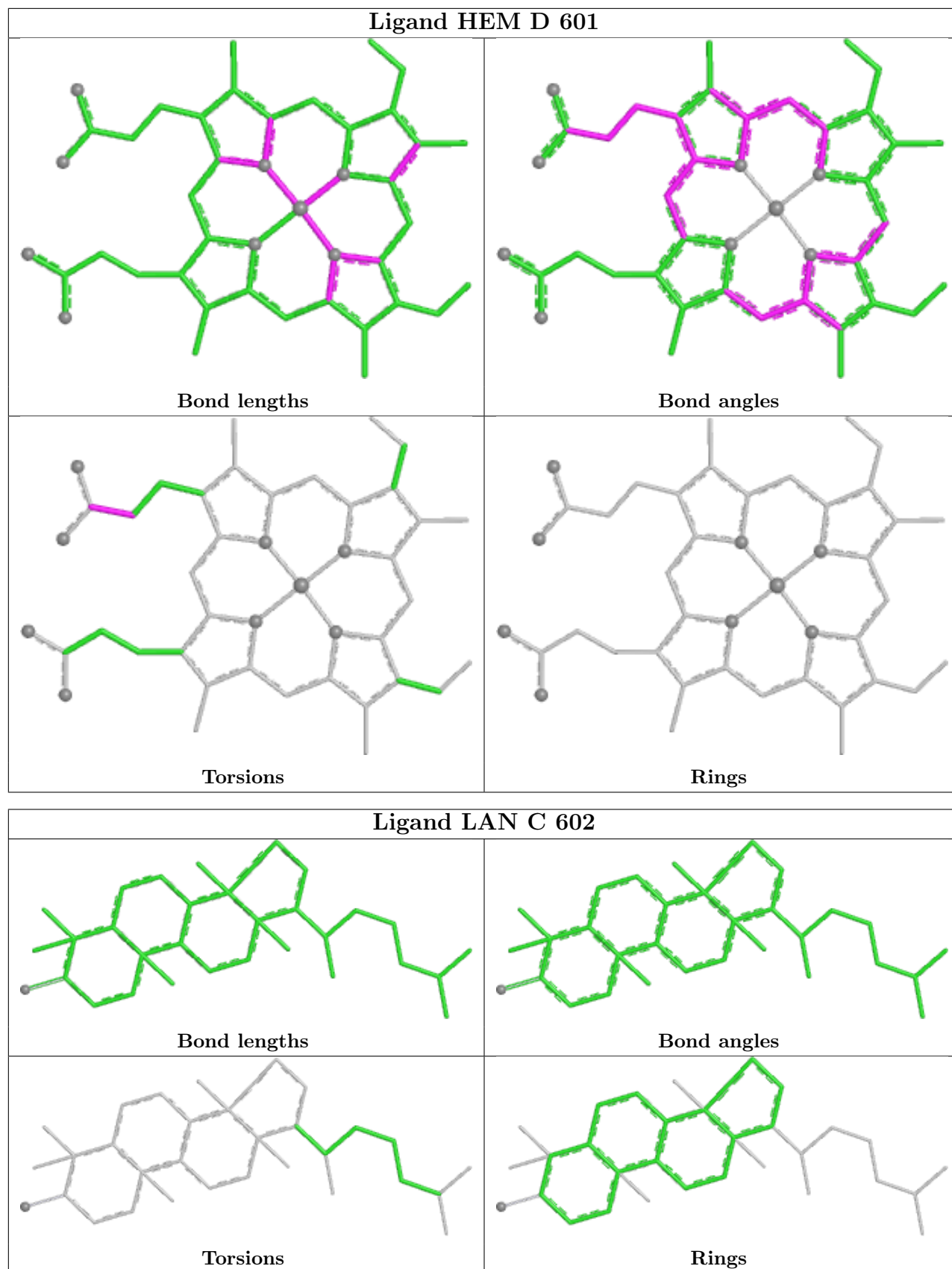
8 monomers are involved in 22 short contacts:

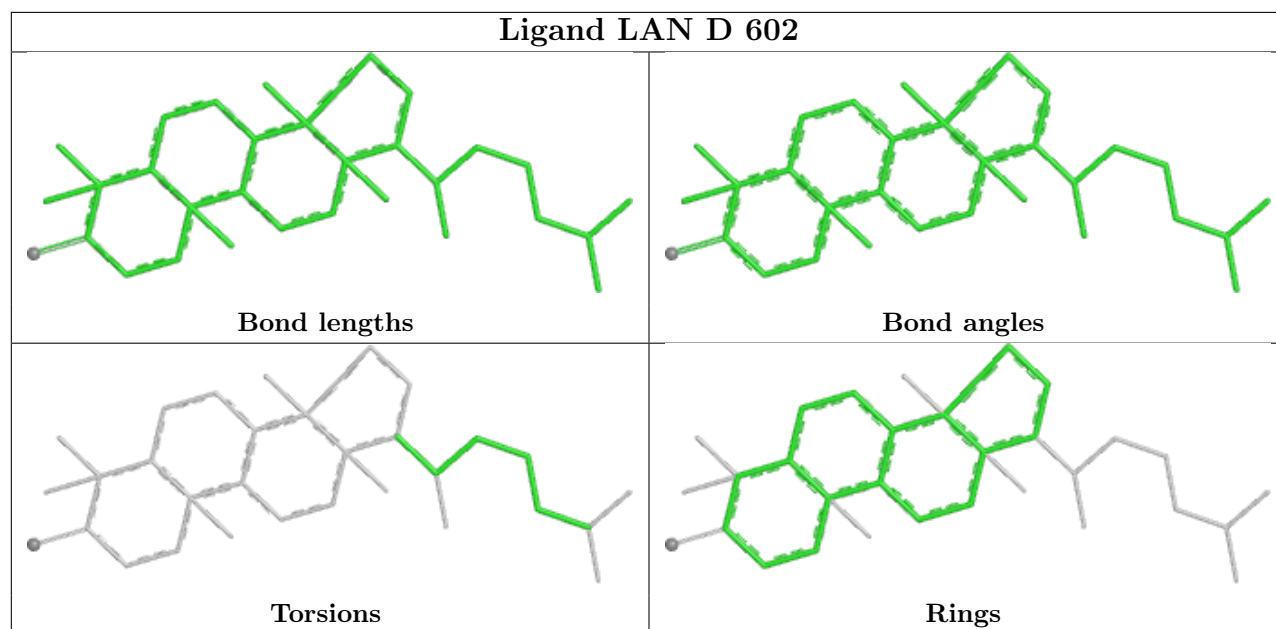
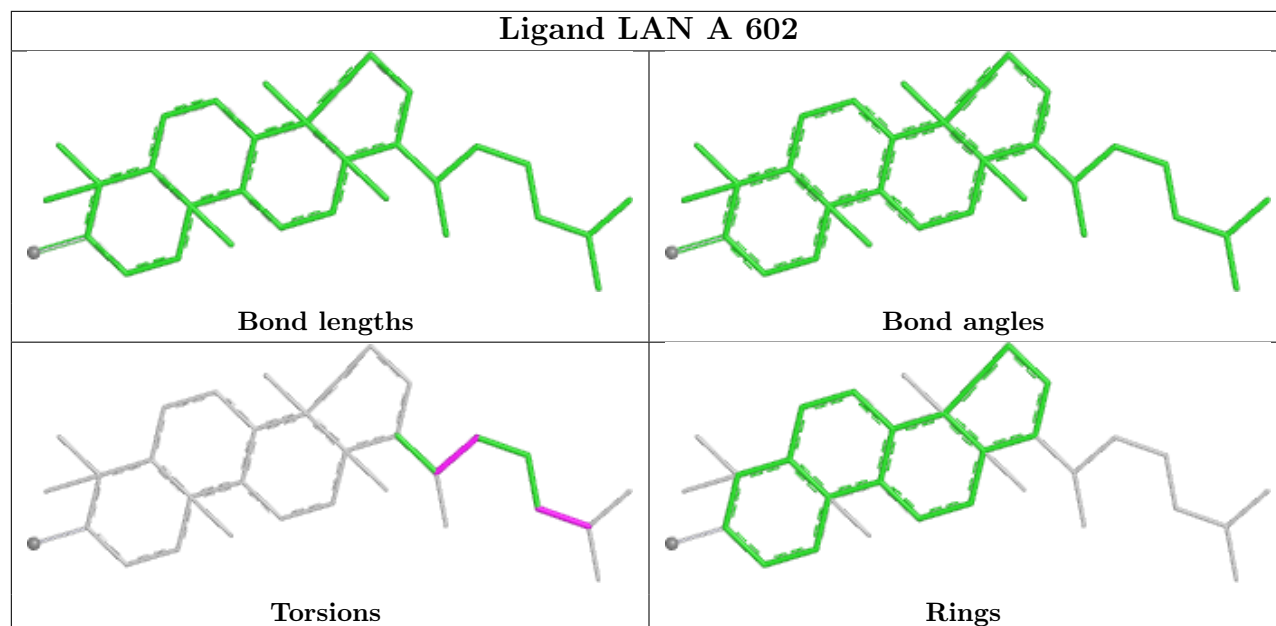
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	1	0
2	A	601	HEM	2	0
2	D	601	HEM	2	0
3	C	602	LAN	4	0
3	A	602	LAN	2	0
3	D	602	LAN	3	0
3	B	602	LAN	5	0
2	B	601	HEM	4	0

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.

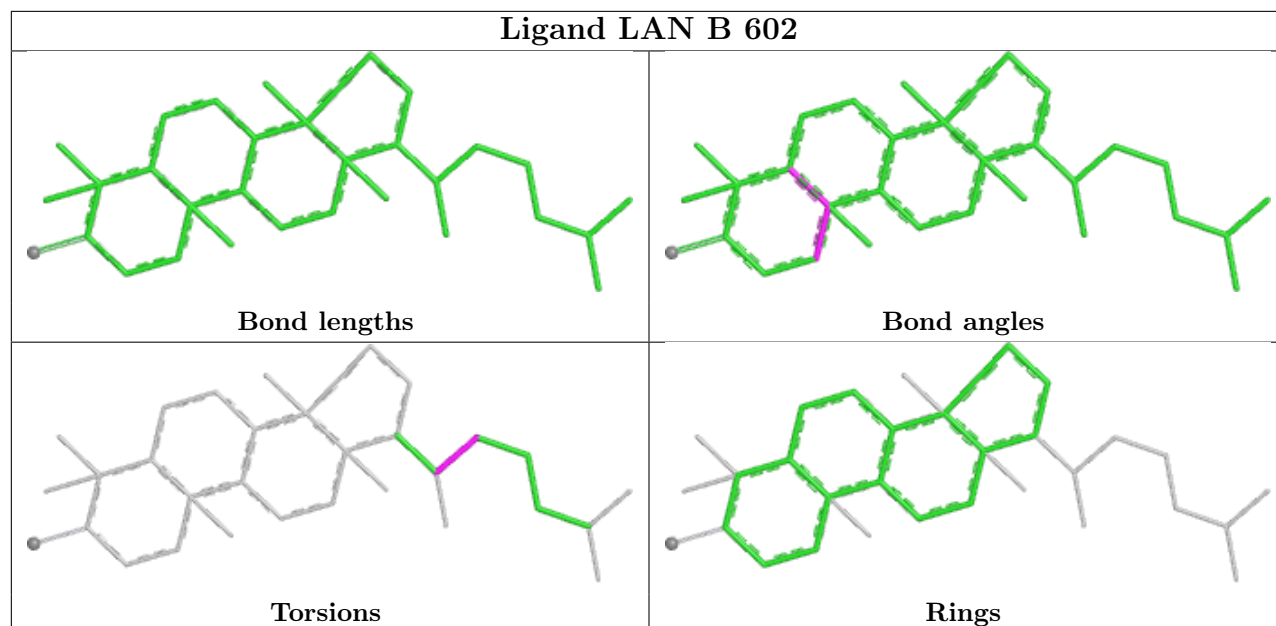




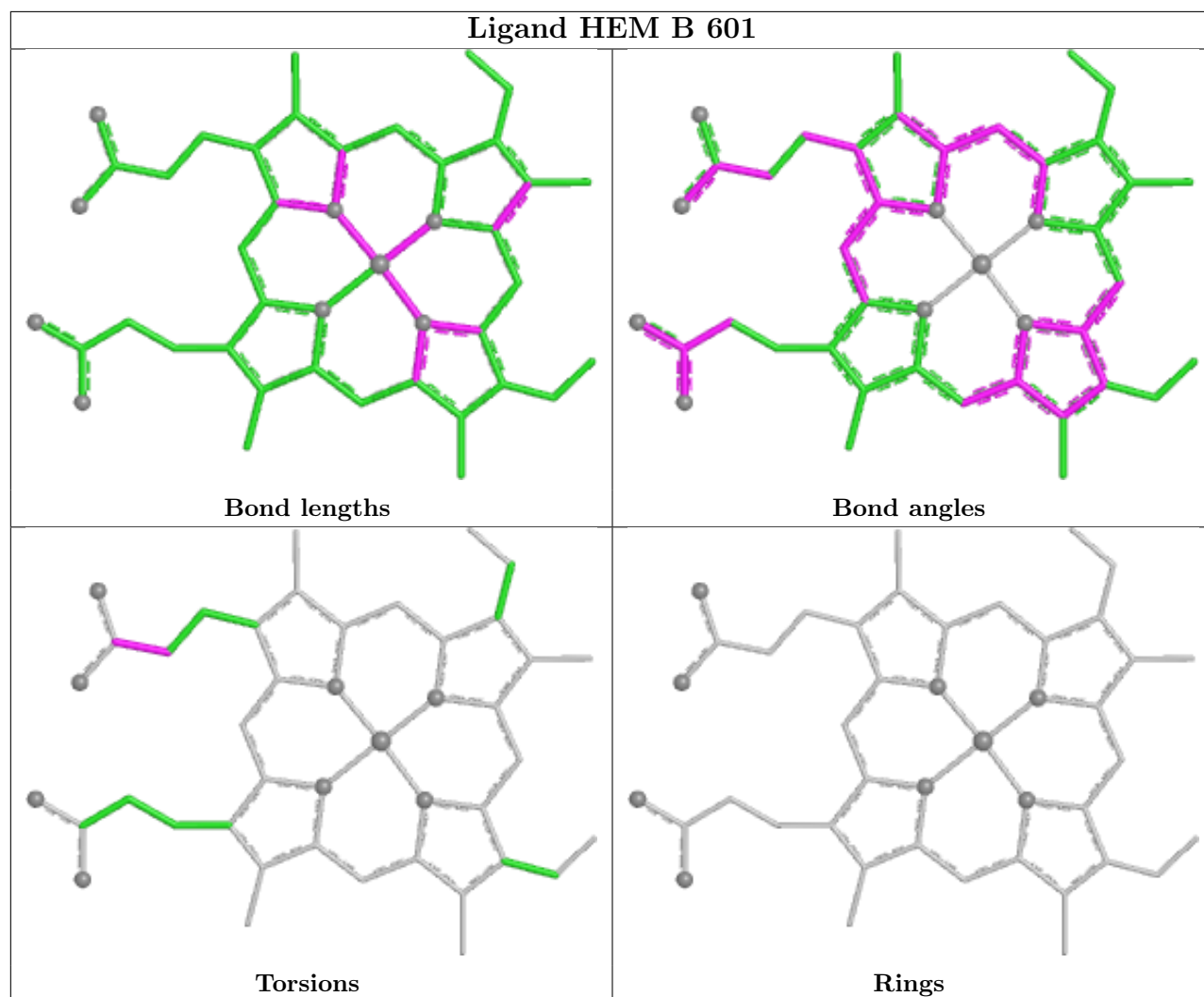




Ligand LAN B 602



Ligand HEM B 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	443/551 (80%)	0.04	16 (3%)	46 47	13, 38, 97, 138	0
1	B	443/551 (80%)	0.18	23 (5%)	33 32	12, 41, 104, 193	0
1	C	440/551 (79%)	0.50	40 (9%)	15 14	16, 55, 144, 172	0
1	D	439/551 (79%)	0.81	69 (15%)	5 4	15, 71, 153, 204	0
All	All	1765/2204 (80%)	0.38	148 (8%)	17 16	12, 51, 132, 204	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	TYR	5.1
1	D	227	VAL	4.9
1	D	297	VAL	4.8
1	B	381	LEU	4.8
1	C	371	TYR	4.6
1	C	409	CYS	4.4
1	B	371	TYR	4.4
1	B	291	PHE	4.3
1	D	381	LEU	4.2
1	D	304	GLN	4.2
1	C	381	LEU	4.2
1	D	106	LEU	4.1
1	A	373	PRO	4.0
1	D	289	ALA	3.9
1	C	373	PRO	3.8
1	D	144	LEU	3.8
1	D	296	ARG	3.6
1	D	373	PRO	3.5
1	C	293	THR	3.5
1	C	139	ILE	3.5
1	C	376	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	3.4
1	B	220	SER	3.3
1	D	307	GLN	3.3
1	D	168	THR	3.3
1	C	379	LYS	3.3
1	B	221	GLN	3.3
1	B	373	PRO	3.3
1	B	225	THR	3.3
1	C	144	LEU	3.2
1	D	218	ALA	3.2
1	A	379	LYS	3.2
1	A	291	PHE	3.1
1	B	165	GLU	3.1
1	C	290	LEU	3.1
1	D	408	VAL	3.1
1	D	170	PHE	3.0
1	D	420	ALA	2.9
1	D	443	ILE	2.9
1	C	374	GLU	2.9
1	D	298	THR	2.9
1	C	423	PRO	2.9
1	C	406	ALA	2.9
1	A	439	SER	2.8
1	D	219	ARG	2.8
1	C	372	THR	2.8
1	D	117	THR	2.8
1	D	379	LYS	2.8
1	C	297	VAL	2.8
1	C	222	GLU	2.8
1	A	226	ASN	2.7
1	C	298	THR	2.7
1	B	222	GLU	2.7
1	B	362	ASN	2.7
1	C	289	ALA	2.7
1	C	420	ALA	2.7
1	A	222	GLU	2.7
1	C	134	LYS	2.7
1	B	219	ARG	2.7
1	D	291	PHE	2.7
1	D	166	LEU	2.7
1	C	291	PHE	2.6
1	C	106	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	225	THR	2.6
1	C	415	TYR	2.6
1	B	233	ASP	2.6
1	D	409	CYS	2.6
1	D	287	ILE	2.6
1	D	448	ARG	2.6
1	A	221	GLN	2.6
1	B	218	ALA	2.6
1	B	379	LYS	2.6
1	C	378	ASP	2.6
1	D	378	ASP	2.6
1	D	376	ALA	2.6
1	D	413	ARG	2.5
1	C	377	GLU	2.5
1	B	226	ASN	2.5
1	B	376	ALA	2.5
1	B	106	LEU	2.5
1	D	293	THR	2.5
1	D	371	TYR	2.5
1	D	113	LYS	2.5
1	D	283	VAL	2.5
1	A	438	ALA	2.5
1	D	234	ALA	2.5
1	C	439	SER	2.5
1	D	214	MET	2.5
1	D	411	LEU	2.5
1	C	299	PHE	2.5
1	D	162	PHE	2.5
1	D	281	ARG	2.5
1	D	230	MET	2.5
1	A	381	LEU	2.4
1	C	413	ARG	2.4
1	B	297	VAL	2.4
1	D	299	PHE	2.4
1	D	375	ARG	2.4
1	D	285	ALA	2.4
1	C	306	PRO	2.4
1	D	439	SER	2.3
1	B	290	LEU	2.3
1	B	378	ASP	2.3
1	D	130	LEU	2.3
1	C	296	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	129	MET	2.3
1	D	422	ALA	2.3
1	D	134	LYS	2.3
1	C	130	LEU	2.3
1	D	415	TYR	2.3
1	D	290	LEU	2.2
1	D	365	LEU	2.2
1	C	135	ASP	2.2
1	D	131	ARG	2.2
1	C	285	ALA	2.2
1	B	113	LYS	2.2
1	C	412	LEU	2.2
1	C	133	TRP	2.2
1	D	167	ASN	2.2
1	C	221	GLN	2.2
1	A	376	ALA	2.2
1	D	382	TYR	2.2
1	D	217	ARG	2.1
1	D	374	GLU	2.1
1	D	110	LEU	2.1
1	B	370	ARG	2.1
1	C	282	ARG	2.1
1	D	111	ARG	2.1
1	D	301	SER	2.1
1	D	114	PRO	2.1
1	D	126	VAL	2.1
1	C	438	ALA	2.1
1	D	295	GLY	2.1
1	C	6	SER	2.1
1	D	370	ARG	2.1
1	D	419	LEU	2.1
1	B	298	THR	2.1
1	D	139	ILE	2.1
1	D	366	PHE	2.0
1	D	231	LEU	2.0
1	A	113	LYS	2.0
1	A	372	THR	2.0
1	D	229	GLN	2.0
1	A	370	ARG	2.0
1	D	402	PHE	2.0
1	D	265	THR	2.0
1	C	301	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	6	SER	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](#)

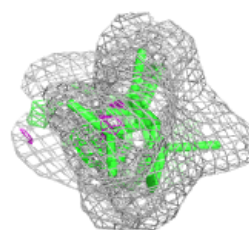
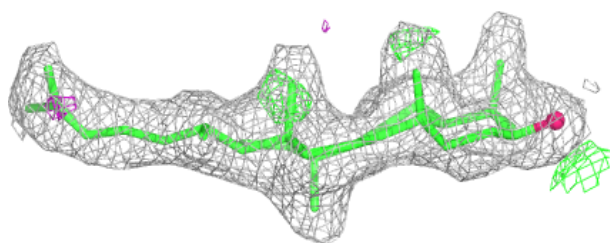
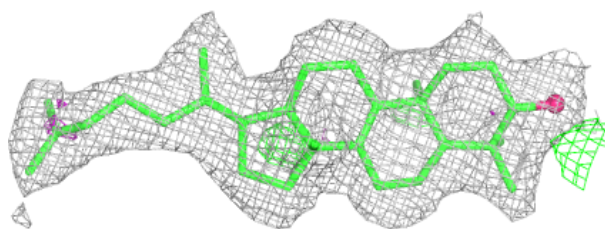
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	LAN	A	602	31/31	0.94	0.08	12,12,19,21	0
3	LAN	C	602	31/31	0.94	0.10	21,26,50,65	0
3	LAN	D	602	31/31	0.94	0.10	24,31,51,69	0
3	LAN	B	602	31/31	0.96	0.08	11,12,60,67	0
2	HEM	D	601	43/43	0.97	0.08	32,40,49,56	0
2	HEM	C	601	43/43	0.98	0.07	27,35,40,41	0
2	HEM	A	601	43/43	0.98	0.06	12,13,16,17	0
2	HEM	B	601	43/43	0.98	0.06	12,15,21,27	0

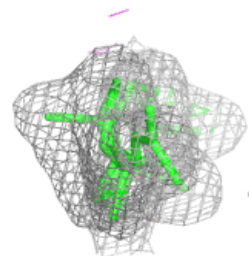
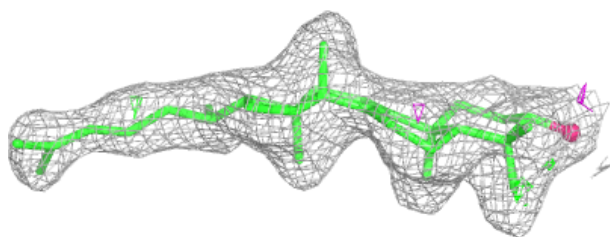
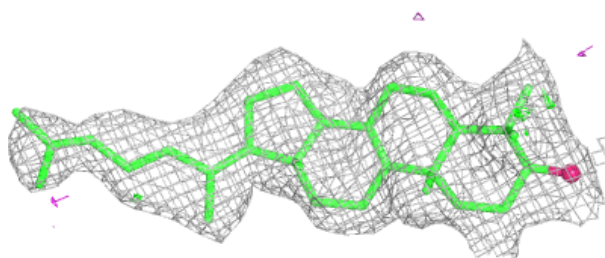
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LAN 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)

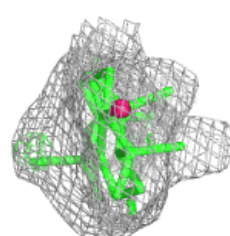
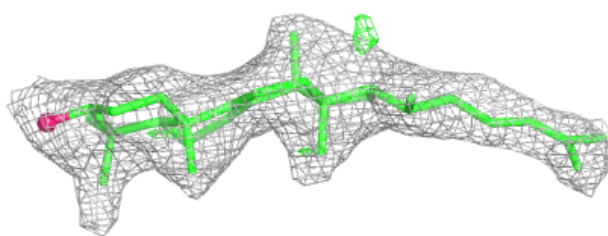
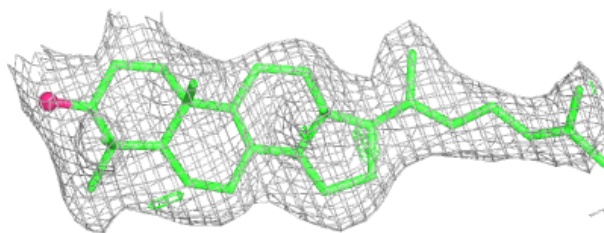
**Electron density around LAN C 602:**

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

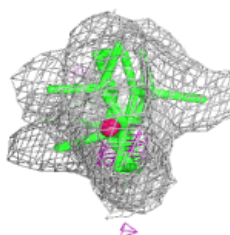
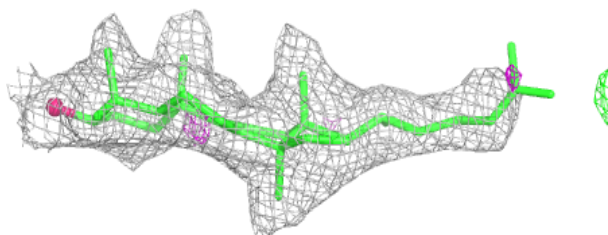
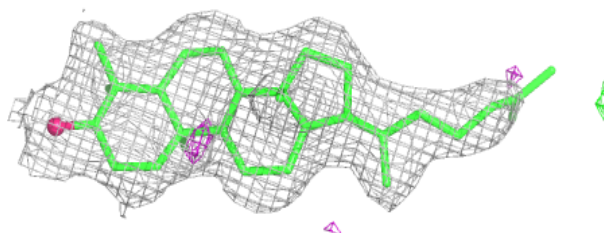


Electron density around LAN D 602:

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

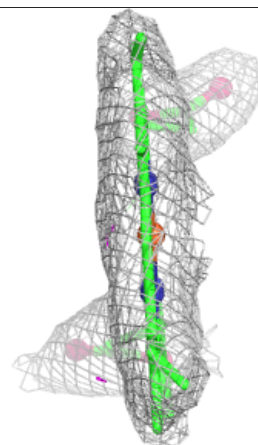
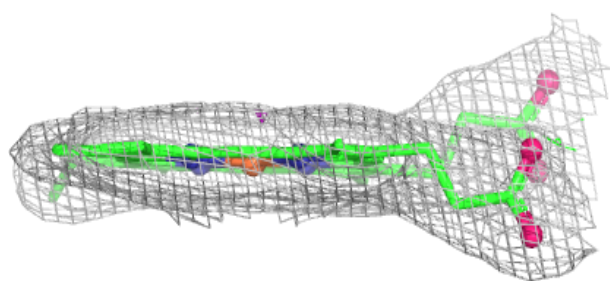
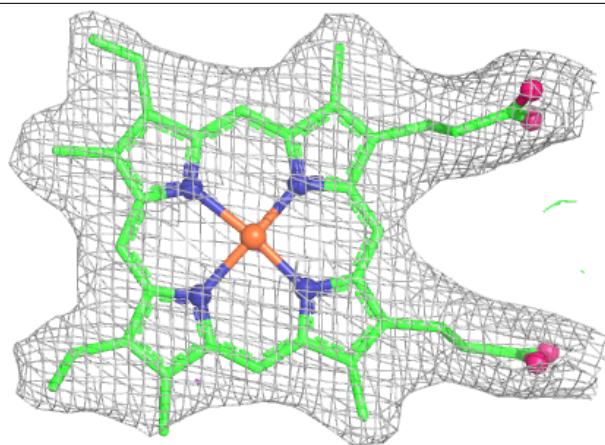
**Electron density around LAN B 602:**

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



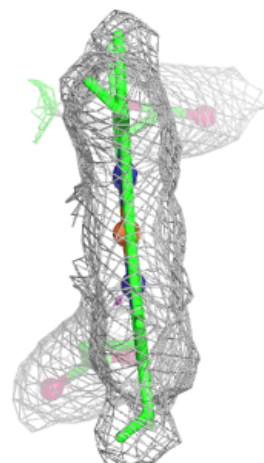
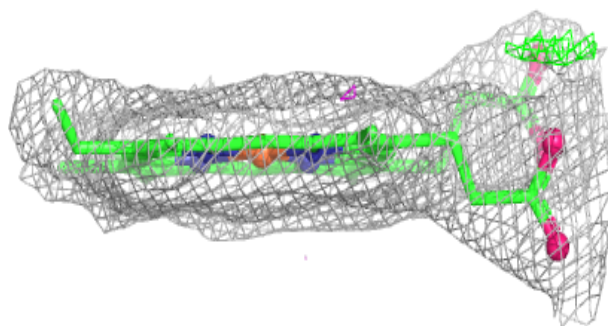
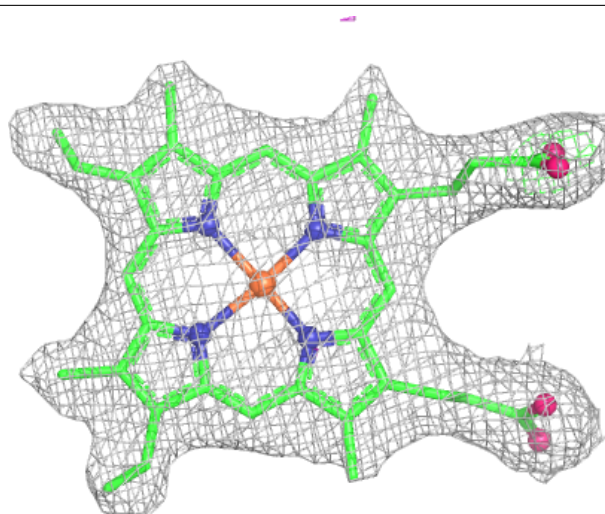
Electron density around HEM D 601:

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



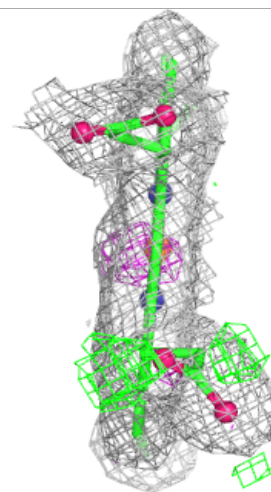
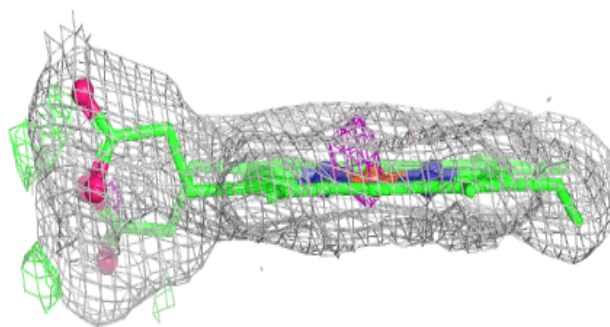
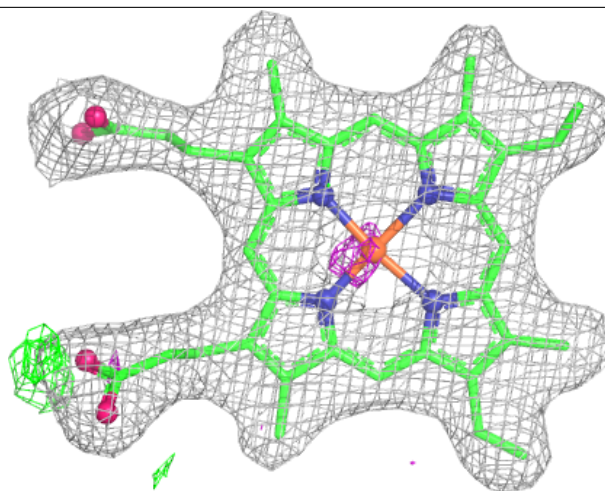
Electron density around HEM C 601:

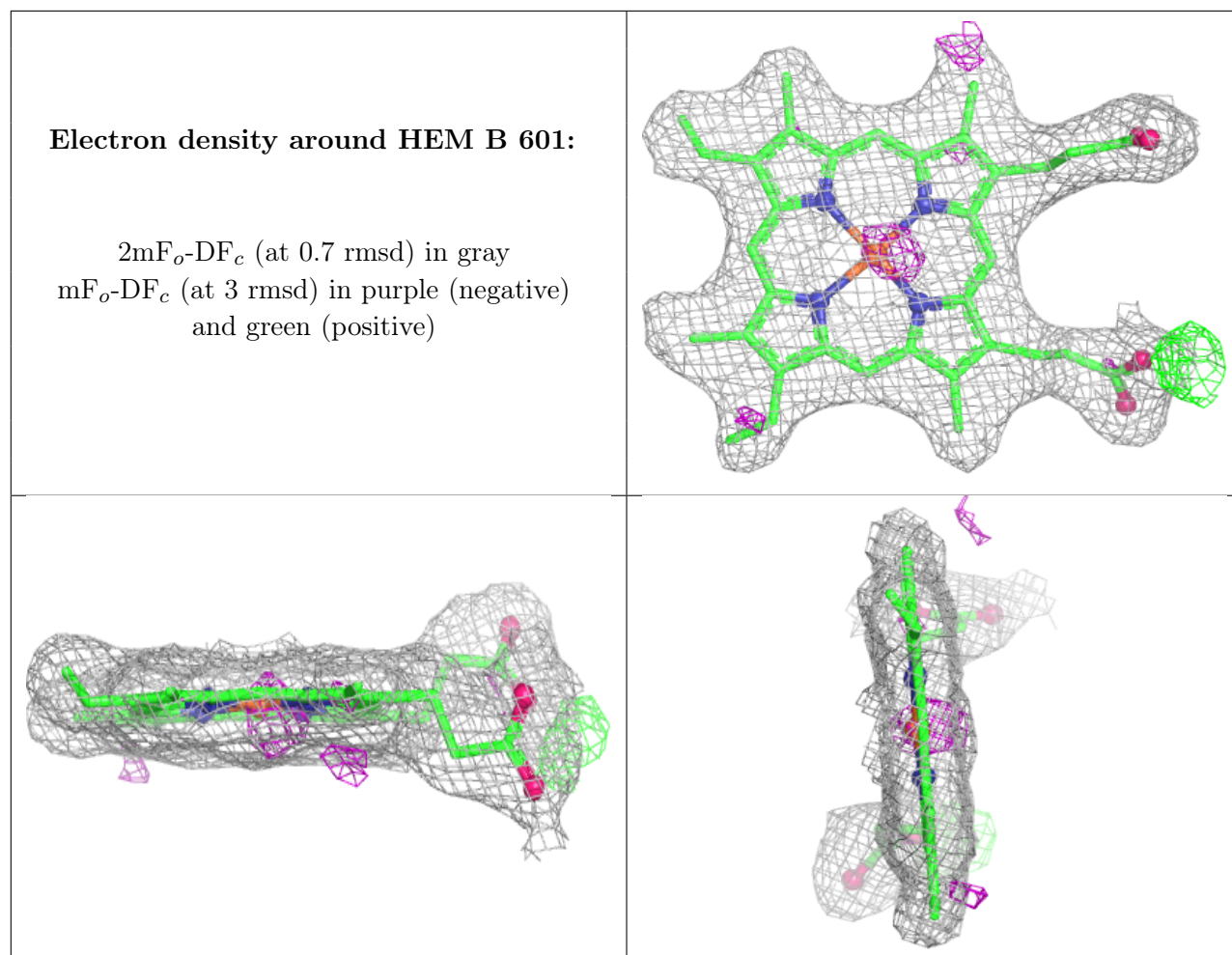
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.