



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:31 PM UTC

PDB ID : 9QLK / pdb_00009qlk
Title : Structure of piperazate synthase from Streptomyces sp.
Authors : Pal, N.; Schroder, S.; Sagmeister, T.; Daniel, B.; Gruber, K.
Deposited on : 2025-03-21
Resolution : 2.14 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

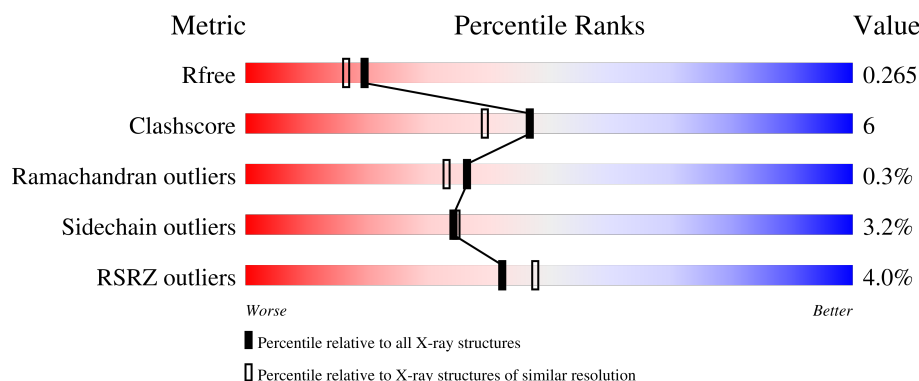
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	229	<div> <div>3%</div> <div>81% 11% 7%</div> </div>
1	B	229	<div> <div>3%</div> <div>84% 7% 7%</div> </div>
1	C	229	<div> <div>2%</div> <div>85% 6% 8%</div> </div>
1	D	229	<div> <div>6%</div> <div>79% 15% 6%</div> </div>
1	E	229	<div> <div>3%</div> <div>79% 13% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	229	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	301	-	-	X	-
3	GOL	D	304	-	-	X	-

2 Entry composition [i](#)

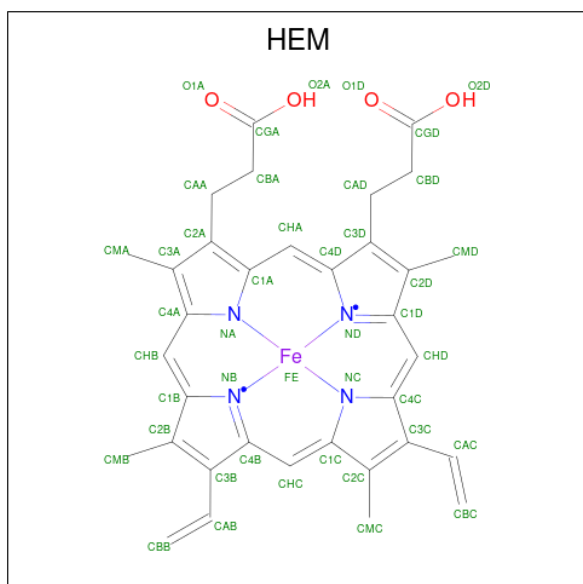
There are 6 unique types of molecules in this entry. The entry contains 20648 atoms, of which 9999 are hydrogens and 0 are deuteriums.

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 FMN-binding negative transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	H	N	O	S	0	0	0
			3274	1048	1615	301	304	6			
1	B	213	Total	C	H	N	O	S	0	2	0
			3319	1060	1641	306	306	6			
1	C	211	Total	C	H	N	O	S	0	1	0
			3280	1053	1619	301	301	6			
1	D	215	Total	C	H	N	O	S	0	3	0
			3369	1079	1664	309	311	6			
1	E	210	Total	C	H	N	O	S	0	0	0
			3243	1037	1603	297	300	6			
1	F	213	Total	C	H	N	O	S	0	1	0
			3298	1055	1628	303	306	6			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

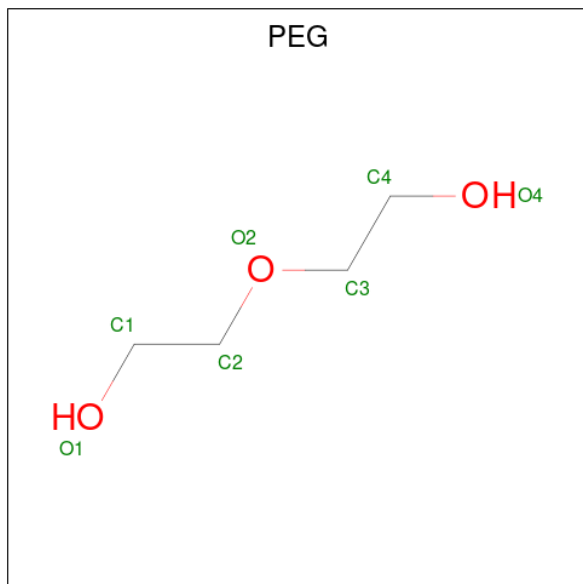


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			17	4	10	3		

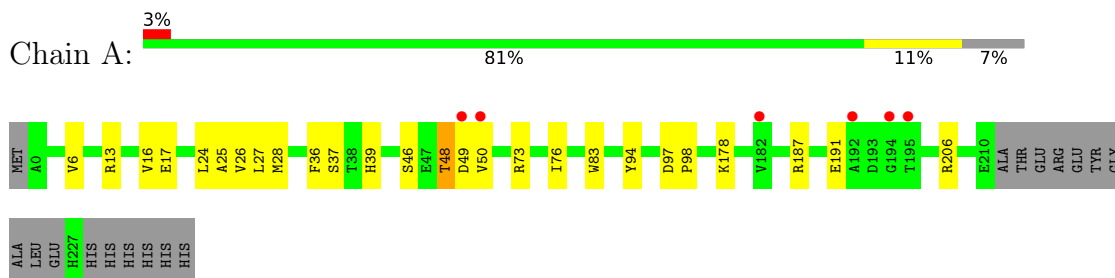
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	62	Total	O	0	0
			62	62		
6	C	53	Total	O	0	0
			53	53		
6	D	48	Total	O	0	0
			48	48		
6	E	59	Total	O	0	0
			59	59		
6	F	50	Total	O	0	0
			50	50		

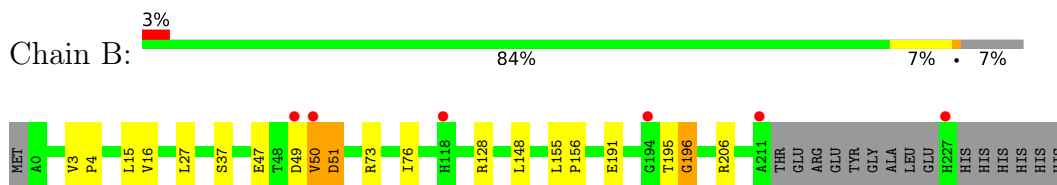
3 Residue-property plots [i](#)

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.

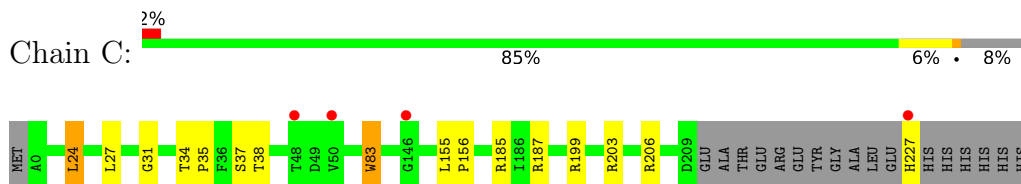
- Molecule 1: FMN-binding negative transcriptional regulator



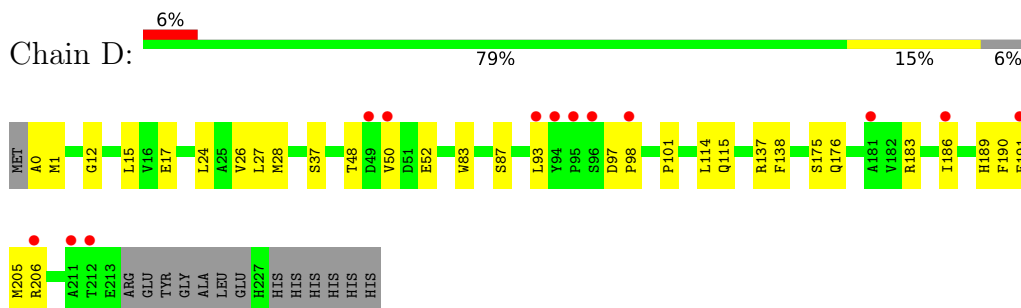
- Molecule 1: FMN-binding negative transcriptional regulator



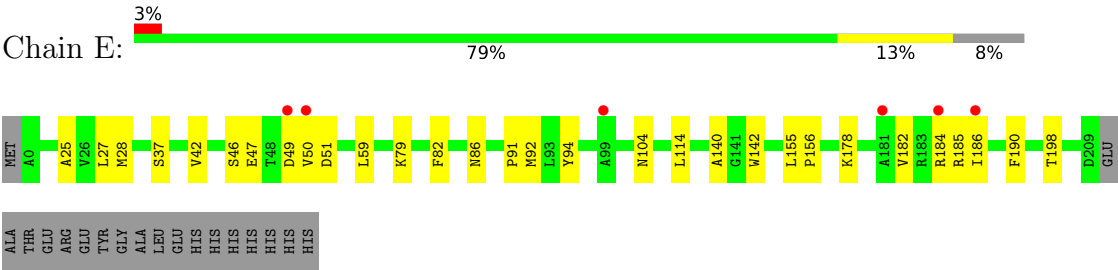
- Molecule 1: FMN-binding negative transcriptional regulator



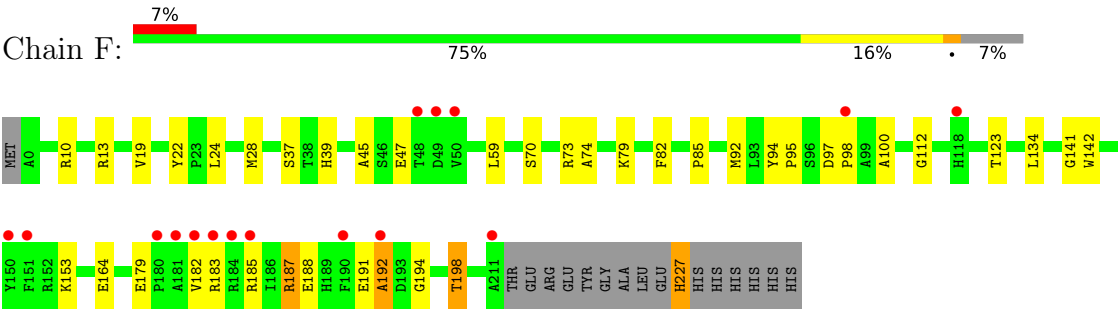
- Molecule 1: FMN-binding negative transcriptional regulator



- Molecule 1: FMN-binding negative transcriptional regulator



● Molecule 1: FMN-binding negative transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	141.71Å 141.71Å 57.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.79 – 2.14 51.79 – 2.14	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.79-2.14) 100.0 (51.79-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.193 , 0.265 0.193 , 0.265	Depositor DCC
R_{free} test set	3541 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.016 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20648	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: PEG, GOL, CA, 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	0.52	0/1703	0.61	0/2317
1	B	0.57	0/1728	0.67	0/2350
1	C	0.58	0/1710	0.68	0/2328
1	D	0.50	0/1760	0.64	0/2395
1	E	0.56	0/1684	0.71	0/2293
1	F	0.52	0/1717	0.66	0/2336
All	All	0.54	0/10302	0.66	0/14019

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	187	ARG	Sidechain

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	1659	1615	1617	14	0
1	B	1678	1641	1643	12	0
1	C	1661	1619	1621	11	0
1	D	1705	1664	1666	26	0
1	E	1640	1603	1605	19	0
1	F	1670	1628	1630	28	0
2	A	43	30	30	3	0
2	B	43	30	30	2	0
2	C	43	30	30	3	0
2	D	43	30	30	2	0
2	E	43	30	30	3	0
2	F	43	30	30	4	0
3	A	6	8	8	0	0
3	C	12	16	16	1	0
3	D	12	15	16	9	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	E	7	10	10	0	0
6	A	66	0	0	0	0
6	B	62	0	0	0	0
6	C	53	0	0	1	0
6	D	48	0	0	0	0
6	E	59	0	0	0	0
6	F	50	0	0	1	0
All	All	10649	9999	10012	115	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 6.

All (115) 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:C:38:THR:HG23	3:D:301:GOL:H31	1.66	0.76
1:F:134:LEU:HD12	2:F:302:HEM:HBB2	1.69	0.75
1:A:13:ARG:HH21	1:A:50:VAL:HG23	1.51	0.75
1:D:48:THR:O	1:D:50:VAL:HG23	1.87	0.74
2:A:301:HEM:HMB2	2:A:301:HEM:HBB2	1.74	0.69
1:F:24:LEU:HD23	1:F:24:LEU:C	2.21	0.65
1:A:26:VAL:HG23	1:A:83:TRP:HZ3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ILE:HG22	1:D:205:MET:HE1	1.78	0.64
1:F:92:MET:HA	1:F:92:MET:HE2	1.81	0.63
2:D:303:HEM:HMB2	2:D:303:HEM:HBB2	1.79	0.62
1:E:92:MET:HE2	1:F:142:TRP:N	2.14	0.61
1:E:50:VAL:HG12	1:E:50:VAL:O	2.02	0.59
2:B:302:HEM:HMB2	2:B:302:HEM:HBB2	1.86	0.57
1:B:51:ASP:N	1:B:51:ASP:OD1	2.37	0.57
1:F:134:LEU:HD12	2:F:302:HEM:CBB	2.34	0.57
1:F:227:HIS:N	1:F:227:HIS:CD2	2.73	0.55
1:F:100:ALA:HB3	1:F:227:HIS:HB3	1.88	0.55
1:A:6:VAL:O	1:A:6:VAL:HG22	2.06	0.55
1:E:92:MET:HE2	1:F:141:GLY:C	2.32	0.55
1:C:24:LEU:HD12	1:D:83[A]:TRP:HH2	1.73	0.54
1:E:91:PRO:HA	1:E:94:TYR:CD2	2.44	0.53
2:A:301:HEM:HBC2	2:A:301:HEM:HHD	1.92	0.52
1:F:123:THR:HG21	6:F:422:HOH:O	2.09	0.52
1:F:183:ARG:O	1:F:187:ARG:HB2	2.10	0.52
1:F:188:GLU:HA	1:F:191:GLU:HB2	1.90	0.52
1:E:86:ASN:HA	1:E:104:ASN:O	2.09	0.52
1:B:15:LEU:N	1:B:15:LEU:HD12	2.25	0.51
1:D:114:LEU:HD23	1:D:115:GLN:N	2.26	0.51
2:F:302:HEM:HBB2	2:F:302:HEM:HMB1	1.93	0.51
1:D:190:PHE:O	1:D:191:GLU:HB2	2.09	0.51
1:E:94:TYR:CE1	1:E:178:LYS:HE3	2.47	0.50
2:E:301:HEM:CMB	2:E:301:HEM:HBB2	2.41	0.50
1:F:191:GLU:O	1:F:192:ALA:O	2.30	0.50
1:D:12:GLY:CA	3:D:304:GOL:H32	2.42	0.49
1:F:28:MET:HE2	1:F:79:LYS:HD2	1.94	0.49
2:D:303:HEM:HBC2	2:D:303:HEM:HHD	1.94	0.49
1:E:28:MET:HE1	1:F:37:SER:HB3	1.93	0.49
1:D:15:LEU:HD22	3:D:304:GOL:H2	1.94	0.49
1:C:24:LEU:HD12	1:D:83[A]:TRP:CH2	2.48	0.48
1:F:24:LEU:HD21	1:F:39:HIS:HB3	1.95	0.48
1:B:27:LEU:O	1:B:37:SER:HA	2.13	0.48
1:D:137:ARG:HD2	1:D:138:PHE:CZ	2.49	0.48
1:F:97:ASP:HB3	1:F:98:PRO:HA	1.96	0.48
1:D:26:VAL:HG23	1:D:83[B]:TRP:HZ3	1.78	0.48
2:A:301:HEM:HBB2	2:A:301:HEM:CMB	2.43	0.47
6:C:404:HOH:O	3:D:301:GOL:H32	2.12	0.47
1:D:186:ILE:CG2	1:D:205:MET:HE1	2.43	0.47
1:E:114:LEU:C	1:E:114:LEU:HD23	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:GLY:HA3	1:F:164:GLU:O	2.14	0.47
1:A:97:ASP:HB3	1:A:98:PRO:HA	1.96	0.47
1:D:97:ASP:HB3	1:D:98:PRO:HA	1.97	0.47
1:E:140:ALA:HB3	1:F:92:MET:HG3	1.96	0.47
1:F:73:ARG:HD2	1:F:74:ALA:O	2.15	0.47
1:D:1:MET:HG3	3:D:301:GOL:H2	1.97	0.46
2:F:302:HEM:HBC2	2:F:302:HEM:HHD	1.98	0.46
1:A:48:THR:O	1:A:50:VAL:HG13	2.15	0.46
1:A:48:THR:O	1:A:50:VAL:N	2.48	0.46
1:E:25:ALA:HB2	1:E:82:PHE:CE2	2.51	0.46
1:F:187:ARG:O	1:F:191:GLU:HG3	2.16	0.45
1:E:50:VAL:O	1:E:50:VAL:CG1	2.65	0.45
1:F:19:VAL:HG13	1:F:82:PHE:CE2	2.50	0.45
1:C:35:PRO:HB2	1:D:28:MET:CE	2.47	0.45
1:A:16:VAL:HG11	1:A:50:VAL:HA	1.98	0.45
1:C:38:THR:HA	3:D:301:GOL:H31	1.99	0.45
1:C:27:LEU:O	1:C:37:SER:HA	2.17	0.45
1:D:52:GLU:OE2	3:D:304:GOL:O2	2.33	0.44
1:D:114:LEU:HD23	1:D:114:LEU:C	2.42	0.44
1:E:142:TRP:HA	1:F:92:MET:HE3	1.99	0.44
1:F:22:TYR:CZ	1:F:85:PRO:HD3	2.53	0.44
1:A:28:MET:HA	1:A:36:PHE:O	2.18	0.44
1:C:155:LEU:N	1:C:156:PRO:CD	2.81	0.44
1:D:50:VAL:O	1:D:50:VAL:HG12	2.18	0.44
1:E:42:VAL:HA	1:E:59:LEU:O	2.18	0.44
1:B:191:GLU:OE2	1:B:206:ARG:NH1	2.51	0.43
1:F:45:ALA:HA	1:F:59:LEU:HD11	1.98	0.43
1:B:50:VAL:HG12	1:B:50:VAL:O	2.17	0.43
1:E:27:LEU:O	1:E:37:SER:HA	2.17	0.43
1:F:179:GLU:HB2	1:F:182:VAL:HG23	2.00	0.43
2:C:301:HEM:CBB	1:D:101:PRO:HB2	2.48	0.43
1:B:155:LEU:N	1:B:156:PRO:CD	2.81	0.43
1:A:27:LEU:O	1:A:37:SER:HA	2.18	0.43
2:E:301:HEM:HBB2	2:E:301:HEM:HMB2	2.00	0.43
2:E:301:HEM:HBC2	2:E:301:HEM:HHD	2.00	0.43
3:C:302:GOL:H12	1:D:0:ALA:N	2.34	0.43
1:D:27:LEU:O	1:D:37:SER:HA	2.19	0.43
1:E:155:LEU:N	1:E:156:PRO:CD	2.82	0.42
1:B:128:ARG:NH2	1:B:148:LEU:HD21	2.35	0.42
1:F:194:GLY:HA3	1:F:198:THR:HG21	2.01	0.42
1:B:16:VAL:HG11	1:B:50:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:HEM:HBB2	2:B:302:HEM:CMB	2.48	0.42
1:A:6:VAL:O	1:A:6:VAL:CG2	2.68	0.42
1:E:92:MET:HE2	1:F:142:TRP:CA	2.50	0.42
2:C:301:HEM:CMB	2:C:301:HEM:HBB2	2.50	0.42
1:C:187:ARG:NH1	1:C:206:ARG:NH2	2.68	0.41
2:C:301:HEM:HBB2	2:C:301:HEM:HMB2	2.01	0.41
1:D:12:GLY:HA3	3:D:304:GOL:H32	2.02	0.41
1:A:25:ALA:O	1:A:39:HIS:HA	2.20	0.41
1:A:187:ARG:O	1:A:191:GLU:HG3	2.21	0.41
1:F:94:TYR:HB3	1:F:95:PRO:HD2	2.02	0.41
1:C:199:ARG:HG2	1:C:203:ARG:HE	1.86	0.41
1:B:195:THR:O	1:B:196:GLY:C	2.63	0.41
1:C:83[A]:TRP:CZ2	1:D:26:VAL:HG23	2.56	0.41
1:D:176:GLN:HA	1:D:183:ARG:HD3	2.03	0.41
1:A:94:TYR:CZ	1:A:178:LYS:HE3	2.56	0.41
1:D:12:GLY:HA2	3:D:304:GOL:C3	2.51	0.41
1:E:186:ILE:HG22	1:E:190:PHE:CE2	2.56	0.41
1:B:3:VAL:HG12	1:B:4:PRO:O	2.20	0.41
1:B:16:VAL:HG11	1:B:50:VAL:HG13	2.02	0.41
1:D:93:LEU:HD21	1:D:189:HIS:HB2	2.03	0.41
1:E:28:MET:CE	1:E:79:LYS:HD2	2.51	0.40
1:B:73:ARG:HG3	1:B:76:ILE:HB	2.03	0.40
1:E:94:TYR:CZ	1:E:178:LYS:HE3	2.56	0.40
1:A:73:ARG:HG2	1:A:76:ILE:HB	2.03	0.40
1:C:31:GLY:HA3	1:C:34:THR:O	2.21	0.40
1:D:87:SER:HB3	1:D:201:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/229 (91%)	198 (95%)	10 (5%)	1 (0%)	24	19
1	B	212/229 (93%)	201 (95%)	9 (4%)	2 (1%)	14	8
1	C	209/229 (91%)	199 (95%)	10 (5%)	0	100	100
1	D	215/229 (94%)	205 (95%)	10 (5%)	0	100	100
1	E	208/229 (91%)	201 (97%)	7 (3%)	0	100	100
1	F	211/229 (92%)	199 (94%)	11 (5%)	1 (0%)	24	19
All	All	1264/1374 (92%)	1203 (95%)	57 (4%)	4 (0%)	36	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	192	ALA
1	A	49	ASP
1	B	50	VAL
1	B	196	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	173/187 (92%)	168 (97%)	5 (3%)	37	38
1	B	175/187 (94%)	172 (98%)	3 (2%)	53	58
1	C	173/187 (92%)	168 (97%)	5 (3%)	37	38
1	D	178/187 (95%)	173 (97%)	5 (3%)	38	39
1	E	171/187 (91%)	163 (95%)	8 (5%)	23	19
1	F	174/187 (93%)	166 (95%)	8 (5%)	24	20
All	All	1044/1122 (93%)	1010 (97%)	34 (3%)	34	33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU

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Mol	Chain	Res	Type
1	A	24	LEU
1	A	46	SER
1	A	48	THR
1	A	206	ARG
1	B	47	GLU
1	B	49	ASP
1	B	51	ASP
1	C	24	LEU
1	C	83[A]	TRP
1	C	83[B]	TRP
1	C	185	ARG
1	C	227	HIS
1	D	17	GLU
1	D	24	LEU
1	D	175	SER
1	D	195	THR
1	D	206	ARG
1	E	46	SER
1	E	47	GLU
1	E	49	ASP
1	E	51	ASP
1	E	182	VAL
1	E	184	ARG
1	E	185	ARG
1	E	198	THR
1	F	10	ARG
1	F	13	ARG
1	F	47	GLU
1	F	70	SER
1	F	153	LYS
1	F	185	ARG
1	F	198	THR
1	F	227	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GOL	D	304	-	5,5,5	0.43	0	5,5,5	0.49	0
3	GOL	C	303	-	5,5,5	0.33	0	5,5,5	0.67	0
5	PEG	E	302	-	6,6,6	0.51	0	5,5,5	0.72	0
2	HEM	B	302	1	50,50,50	1.56	7 (14%)	67,82,82	1.18	5 (7%)
3	GOL	A	302	-	5,5,5	0.27	0	5,5,5	0.80	0
3	GOL	C	302	-	5,5,5	0.32	0	5,5,5	0.41	0
2	HEM	C	301	1	50,50,50	1.58	8 (16%)	67,82,82	1.27	6 (8%)
2	HEM	F	302	1,6	50,50,50	1.83	9 (18%)	67,82,82	1.59	15 (22%)
2	HEM	E	301	1	50,50,50	1.53	10 (20%)	67,82,82	1.04	2 (2%)
3	GOL	D	301	-	5,5,5	0.64	0	5,5,5	0.69	0
2	HEM	A	301	1	50,50,50	1.35	6 (12%)	67,82,82	1.30	10 (14%)
2	HEM	D	303	1	50,50,50	1.64	7 (14%)	67,82,82	1.40	12 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	304	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	303	-	-	4/4/4/4	-
5	PEG	E	302	-	-	0/4/4/4	-
2	HEM	B	302	1	-	5/14/54/54	-
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	C	302	-	-	2/4/4/4	-
2	HEM	C	301	1	-	5/14/54/54	-
2	HEM	F	302	1,6	-	5/14/54/54	-
2	HEM	E	301	1	-	5/14/54/54	-
3	GOL	D	301	-	-	4/4/4/4	-
2	HEM	A	301	1	-	4/14/54/54	-
2	HEM	D	303	1	-	3/14/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	303	HEM	FE-NC	6.27	2.15	1.95
2	F	302	HEM	FE-NC	6.17	2.15	1.95
2	B	302	HEM	FE-NC	5.59	2.13	1.95
2	F	302	HEM	FE-ND	5.52	2.11	1.94
2	E	301	HEM	FE-NC	4.64	2.10	1.95
2	C	301	HEM	FE-NB	4.59	2.09	1.94
2	C	301	HEM	FE-ND	4.04	2.07	1.94
2	F	302	HEM	FE-NA	3.90	2.08	1.95
2	D	303	HEM	FE-NA	3.81	2.07	1.95
2	F	302	HEM	CAB-C3B	3.78	1.57	1.47
2	D	303	HEM	CAB-C3B	3.64	1.57	1.47
2	A	301	HEM	FE-NA	3.48	2.06	1.95
2	A	301	HEM	FE-NC	3.47	2.06	1.95
2	F	302	HEM	FE-NB	3.45	2.05	1.94
2	B	302	HEM	CAB-C3B	3.31	1.56	1.47
2	E	301	HEM	CAB-C3B	3.28	1.56	1.47
2	D	303	HEM	FE-NB	3.22	2.04	1.94
2	C	301	HEM	CMD-C2D	3.15	1.57	1.50
2	C	301	HEM	CAC-C3C	3.07	1.55	1.47
2	B	302	HEM	FE-NB	2.99	2.04	1.94
2	A	301	HEM	CAC-C3C	2.88	1.55	1.47
2	C	301	HEM	FE-NA	2.84	2.04	1.95
2	D	303	HEM	CAC-C3C	2.82	1.54	1.47
2	C	301	HEM	CAB-C3B	2.77	1.54	1.47
2	E	301	HEM	FE-NB	-2.73	1.86	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	HEM	FE-NA	2.72	2.04	1.95
2	A	301	HEM	CAB-C3B	2.64	1.54	1.47
2	C	301	HEM	FE-NC	2.63	2.03	1.95
2	F	302	HEM	CAC-C3C	2.62	1.54	1.47
2	B	302	HEM	C2A-C3A	-2.61	1.32	1.38
2	B	302	HEM	CAC-C3C	2.59	1.54	1.47
2	D	303	HEM	CMB-C2B	2.51	1.55	1.50
2	E	301	HEM	CMD-C2D	2.40	1.55	1.50
2	D	303	HEM	CMD-C2D	2.32	1.55	1.50
2	F	302	HEM	CMA-C3A	2.30	1.55	1.50
2	F	302	HEM	CMD-C2D	2.28	1.55	1.50
2	C	301	HEM	CMB-C2B	2.25	1.55	1.50
2	B	302	HEM	CMB-C2B	2.25	1.55	1.50
2	E	301	HEM	CMA-C3A	2.23	1.55	1.50
2	E	301	HEM	C2A-C3A	-2.21	1.33	1.38
2	E	301	HEM	CAC-C3C	2.18	1.53	1.47
2	A	301	HEM	CMA-C3A	2.10	1.55	1.50
2	A	301	HEM	CMC-C2C	2.10	1.55	1.50
2	E	301	HEM	CMC-C2C	2.10	1.55	1.50
2	E	301	HEM	CMB-C2B	2.06	1.55	1.50
2	F	302	HEM	CMC-C2C	2.05	1.55	1.50
2	E	301	HEM	C3B-C2B	-2.02	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	302	HEM	C3B-C2B-C1B	4.10	109.49	106.41
2	F	302	HEM	C4D-ND-C1D	4.02	109.96	105.21
2	C	301	HEM	C2A-C1A-NA	-3.60	106.16	110.15
2	F	302	HEM	C2A-C1A-NA	-3.39	106.39	110.15
2	D	303	HEM	CHC-C4B-NB	3.36	128.04	124.42
2	E	301	HEM	CHC-C4B-NB	3.35	128.03	124.42
2	D	303	HEM	CHD-C1D-ND	3.25	127.92	124.42
2	A	301	HEM	CHD-C1D-ND	3.18	127.85	124.42
2	F	302	HEM	CHD-C1D-ND	3.13	127.79	124.42
2	F	302	HEM	C2D-C1D-ND	-3.04	106.39	109.90
2	F	302	HEM	C4A-NA-C1A	2.96	110.64	105.82
2	F	302	HEM	C3D-C4D-ND	-2.90	106.99	110.17
2	F	302	HEM	CAD-CBD-CGD	-2.89	105.99	113.67
2	C	301	HEM	C4D-ND-C1D	2.84	108.58	105.21
2	B	302	HEM	CHD-C1D-ND	2.80	127.44	124.42
2	D	303	HEM	C3B-C2B-C1B	2.71	108.45	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	303	HEM	C4A-C3A-C2A	2.61	109.81	106.82
2	C	301	HEM	C3D-C4D-ND	-2.56	107.36	110.17
2	A	301	HEM	CHB-C1B-NB	2.50	127.46	124.37
2	B	302	HEM	C3B-C2B-C1B	2.48	108.27	106.41
2	D	303	HEM	O1D-CGD-CBD	-2.47	115.25	123.09
2	A	301	HEM	C2A-C1A-NA	-2.41	107.48	110.15
2	A	301	HEM	C1D-C2D-C3D	2.40	109.51	106.98
2	F	302	HEM	C2B-C1B-NB	-2.40	107.08	109.84
2	A	301	HEM	CAD-CBD-CGD	-2.39	107.32	113.67
2	B	302	HEM	C4A-C3A-C2A	2.33	109.48	106.82
2	D	303	HEM	CHD-C4C-C3C	2.31	129.11	125.21
2	B	302	HEM	C3A-C4A-NA	-2.30	106.45	110.14
2	D	303	HEM	C3A-C4A-NA	-2.29	106.47	110.14
2	F	302	HEM	C1B-NB-C4B	2.29	107.91	105.21
2	A	301	HEM	C2D-C1D-ND	-2.28	107.27	109.90
2	D	303	HEM	CMA-C3A-C4A	-2.26	121.98	125.42
2	F	302	HEM	C3A-C4A-NA	-2.25	106.54	110.14
2	C	301	HEM	C1B-NB-C4B	2.24	107.86	105.21
2	C	301	HEM	C4A-NA-C1A	2.21	109.42	105.82
2	A	301	HEM	C4D-ND-C1D	2.18	107.79	105.21
2	F	302	HEM	CHA-C4D-C3D	2.14	129.18	125.23
2	A	301	HEM	C3C-C2C-C1C	2.13	109.06	107.05
2	A	301	HEM	CHA-C4D-ND	2.11	126.97	124.37
2	E	301	HEM	CHD-C1D-ND	2.08	126.67	124.42
2	F	302	HEM	CHD-C4C-C3C	2.08	128.72	125.21
2	D	303	HEM	C4A-NA-C1A	2.08	109.21	105.82
2	D	303	HEM	C2B-C1B-NB	-2.08	107.45	109.84
2	B	302	HEM	C4D-ND-C1D	2.07	107.66	105.21
2	D	303	HEM	O2A-CGA-CBA	2.07	120.54	114.00
2	C	301	HEM	CHC-C1C-NC	2.07	126.70	124.45
2	F	302	HEM	C4C-NC-C1C	2.05	109.17	105.82
2	F	302	HEM	CAD-C3D-C2D	-2.01	124.10	127.87
2	A	301	HEM	C3B-C2B-C1B	2.01	107.92	106.41
2	D	303	HEM	O2D-CGD-CBD	2.00	120.33	114.00

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	C	302	GOL	C1-C2-C3-O3
3	C	303	GOL	O1-C1-C2-C3

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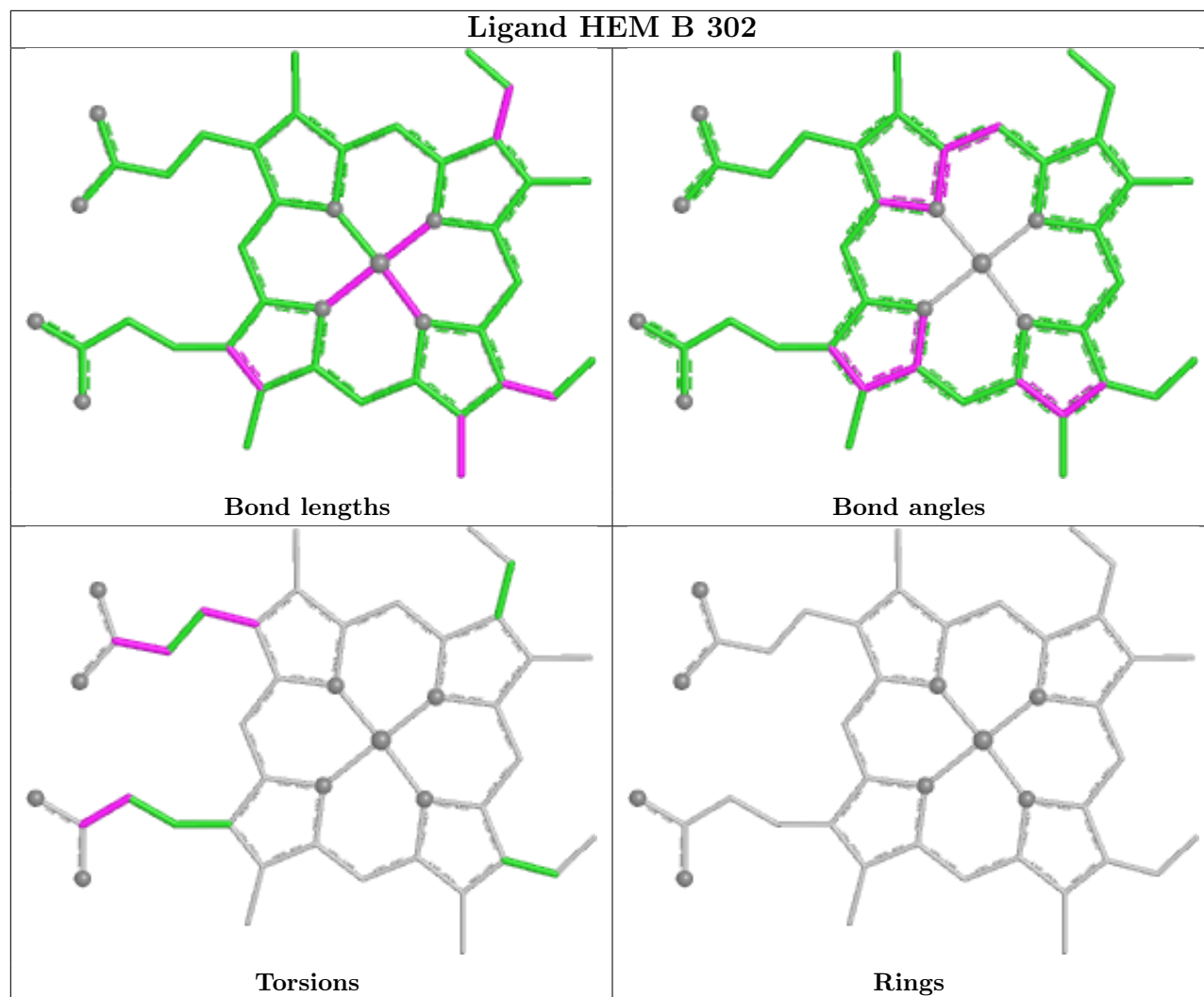
Mol	Chain	Res	Type	Atoms
3	D	304	GOL	O1-C1-C2-O2
2	E	301	HEM	C3D-CAD-CBD-CGD
3	A	302	GOL	O2-C2-C3-O3
3	C	303	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-C3
3	D	301	GOL	C1-C2-C3-O3
3	D	304	GOL	O1-C1-C2-C3
3	C	302	GOL	O2-C2-C3-O3
3	C	303	GOL	O1-C1-C2-O2
3	D	301	GOL	O2-C2-C3-O3
3	C	303	GOL	O2-C2-C3-O3
3	D	301	GOL	O1-C1-C2-O2
2	F	302	HEM	C3D-CAD-CBD-CGD
2	D	303	HEM	C2D-C3D-CAD-CBD
2	D	303	HEM	C4D-C3D-CAD-CBD
2	E	301	HEM	CAA-CBA-CGA-O2A
2	A	301	HEM	CAA-CBA-CGA-O1A
2	E	301	HEM	CAD-CBD-CGD-O2D
2	E	301	HEM	CAA-CBA-CGA-O1A
2	F	302	HEM	CAA-CBA-CGA-O1A
2	F	302	HEM	CAD-CBD-CGD-O1D
2	F	302	HEM	CAD-CBD-CGD-O2D
2	E	301	HEM	CAD-CBD-CGD-O1D
2	F	302	HEM	CAA-CBA-CGA-O2A
2	B	302	HEM	CAA-CBA-CGA-O1A
2	C	301	HEM	CAA-CBA-CGA-O1A
2	C	301	HEM	C2D-C3D-CAD-CBD
2	A	301	HEM	CAA-CBA-CGA-O2A
2	B	302	HEM	CAA-CBA-CGA-O2A
2	C	301	HEM	CAA-CBA-CGA-O2A
2	B	302	HEM	CAD-CBD-CGD-O2D
2	B	302	HEM	C2D-C3D-CAD-CBD
2	B	302	HEM	CAD-CBD-CGD-O1D
2	A	301	HEM	C4D-C3D-CAD-CBD
2	A	301	HEM	C2D-C3D-CAD-CBD
2	C	301	HEM	CAD-CBD-CGD-O2D
2	C	301	HEM	CAD-CBD-CGD-O1D
2	D	303	HEM	CAA-CBA-CGA-O1A

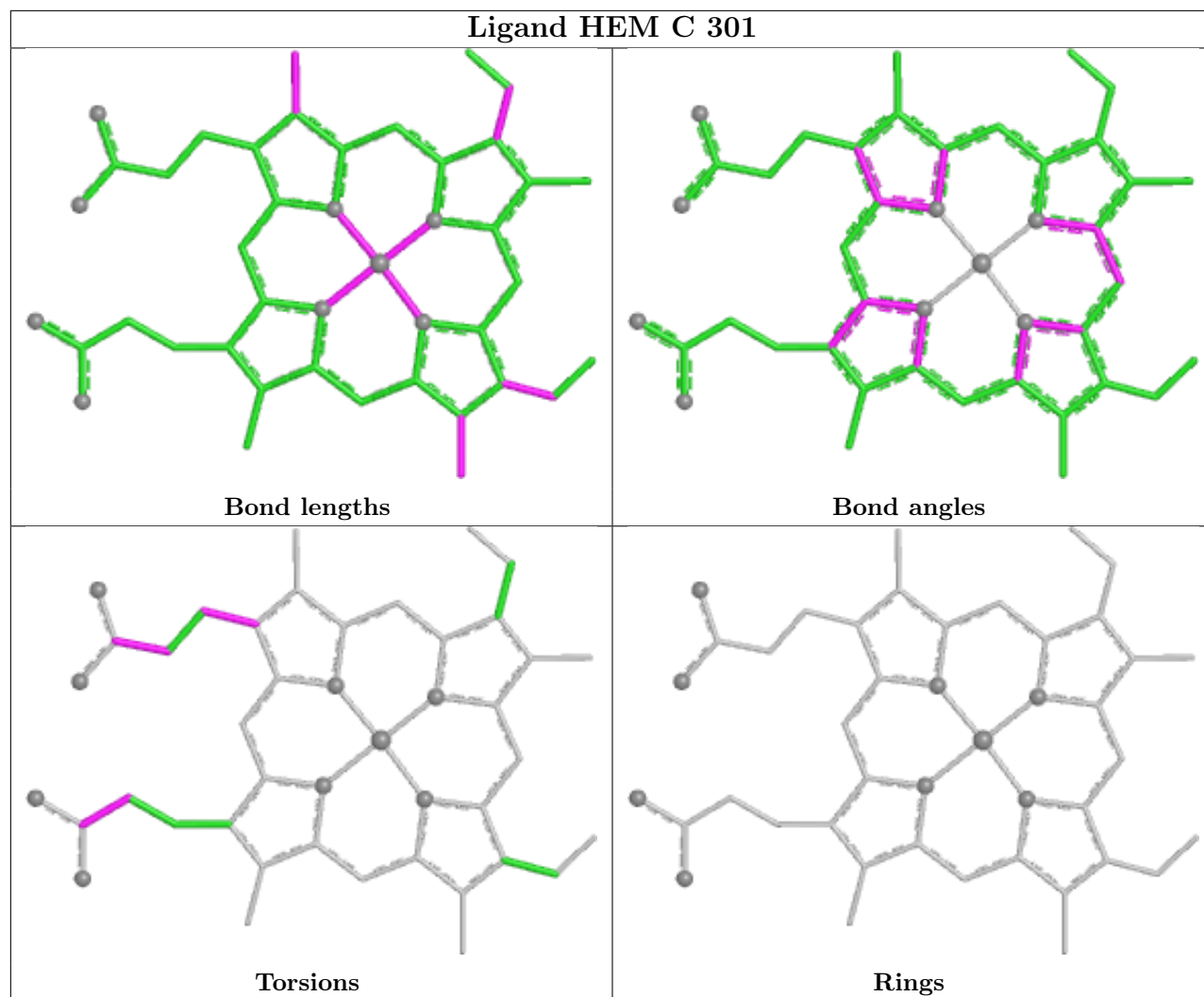
There are no ring outliers.

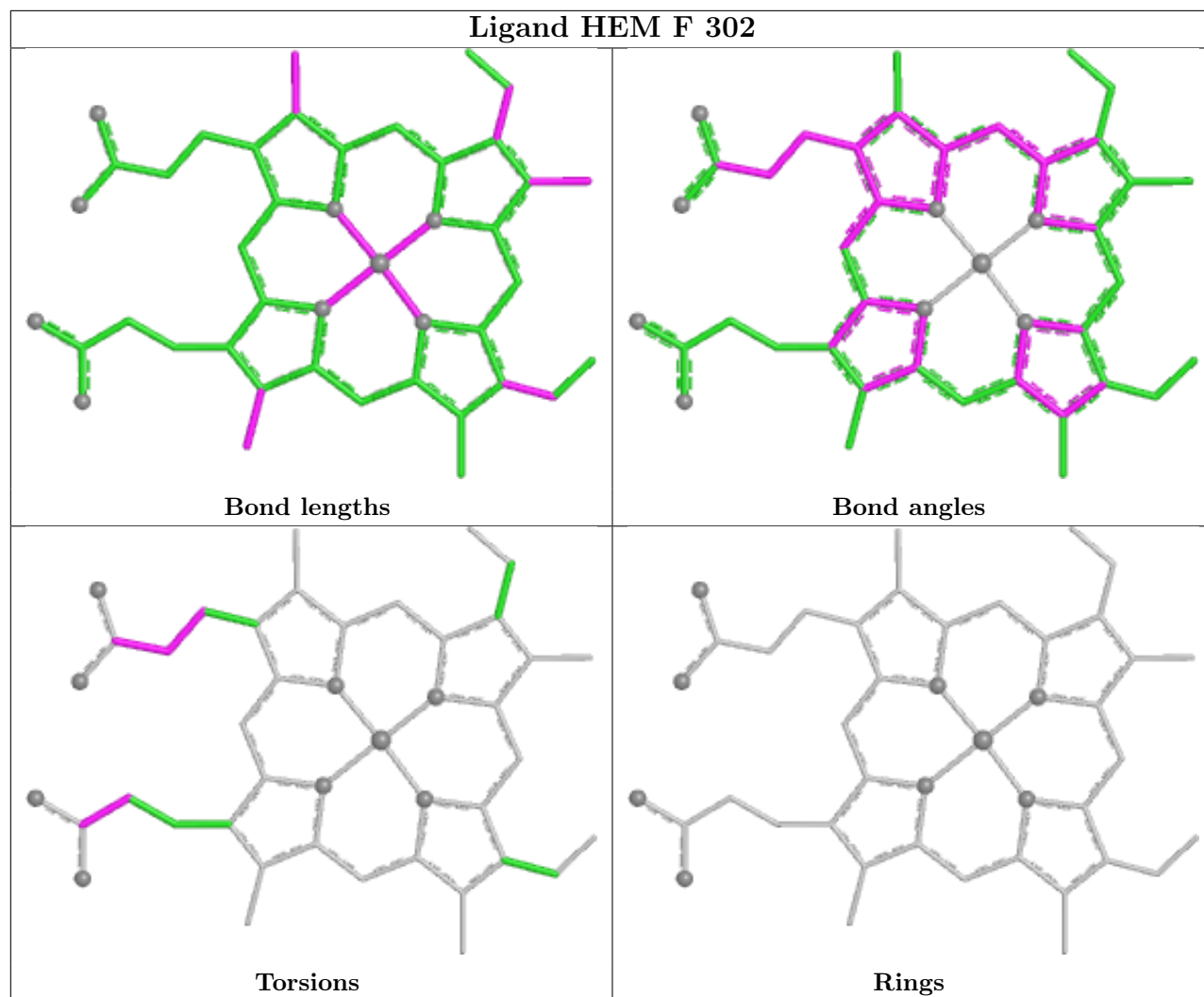
9 monomers are involved in 27 short contacts:

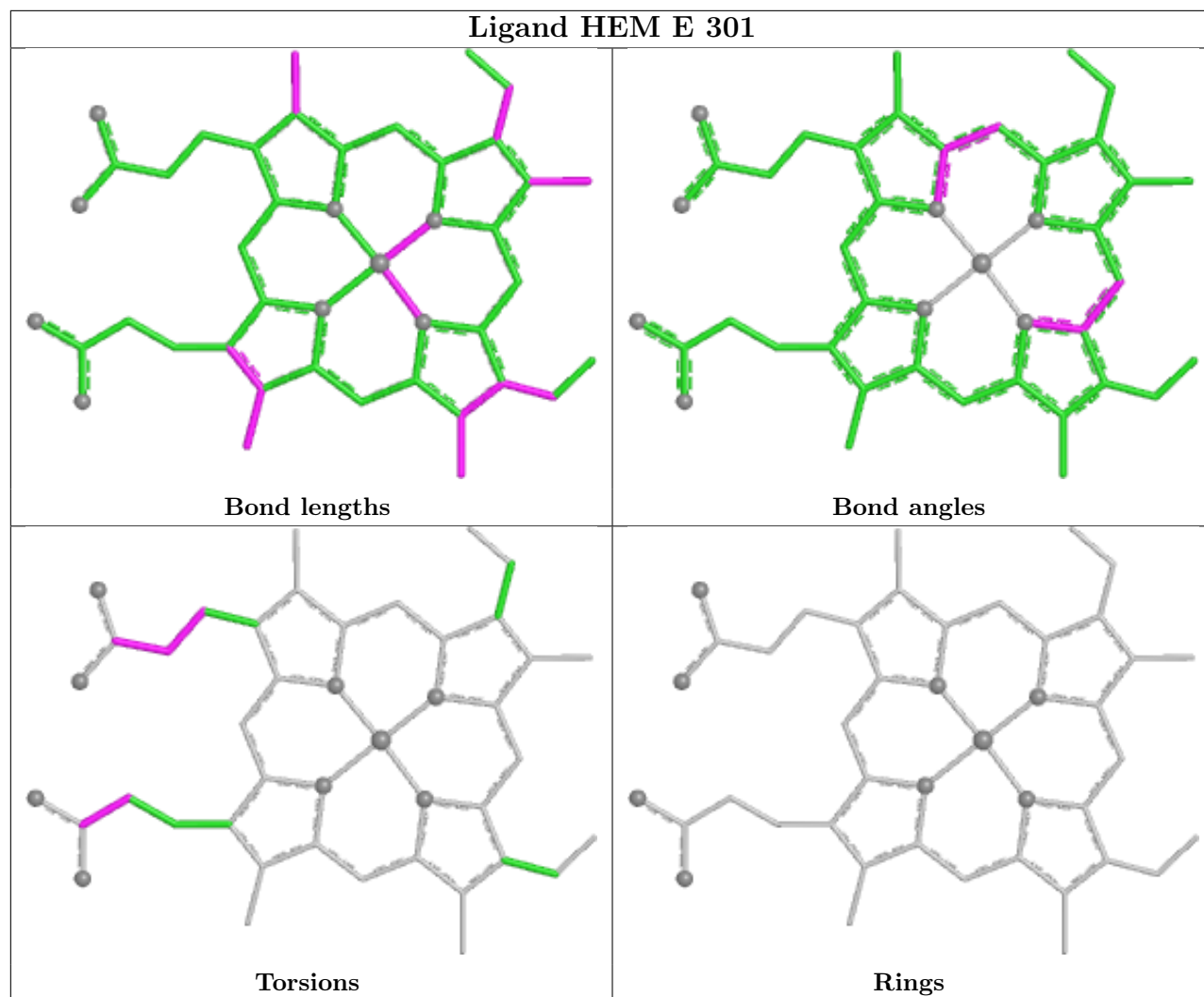
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	304	GOL	5	0
2	B	302	HEM	2	0
3	C	302	GOL	1	0
2	C	301	HEM	3	0
2	F	302	HEM	4	0
2	E	301	HEM	3	0
3	D	301	GOL	4	0
2	A	301	HEM	3	0
2	D	303	HEM	2	0

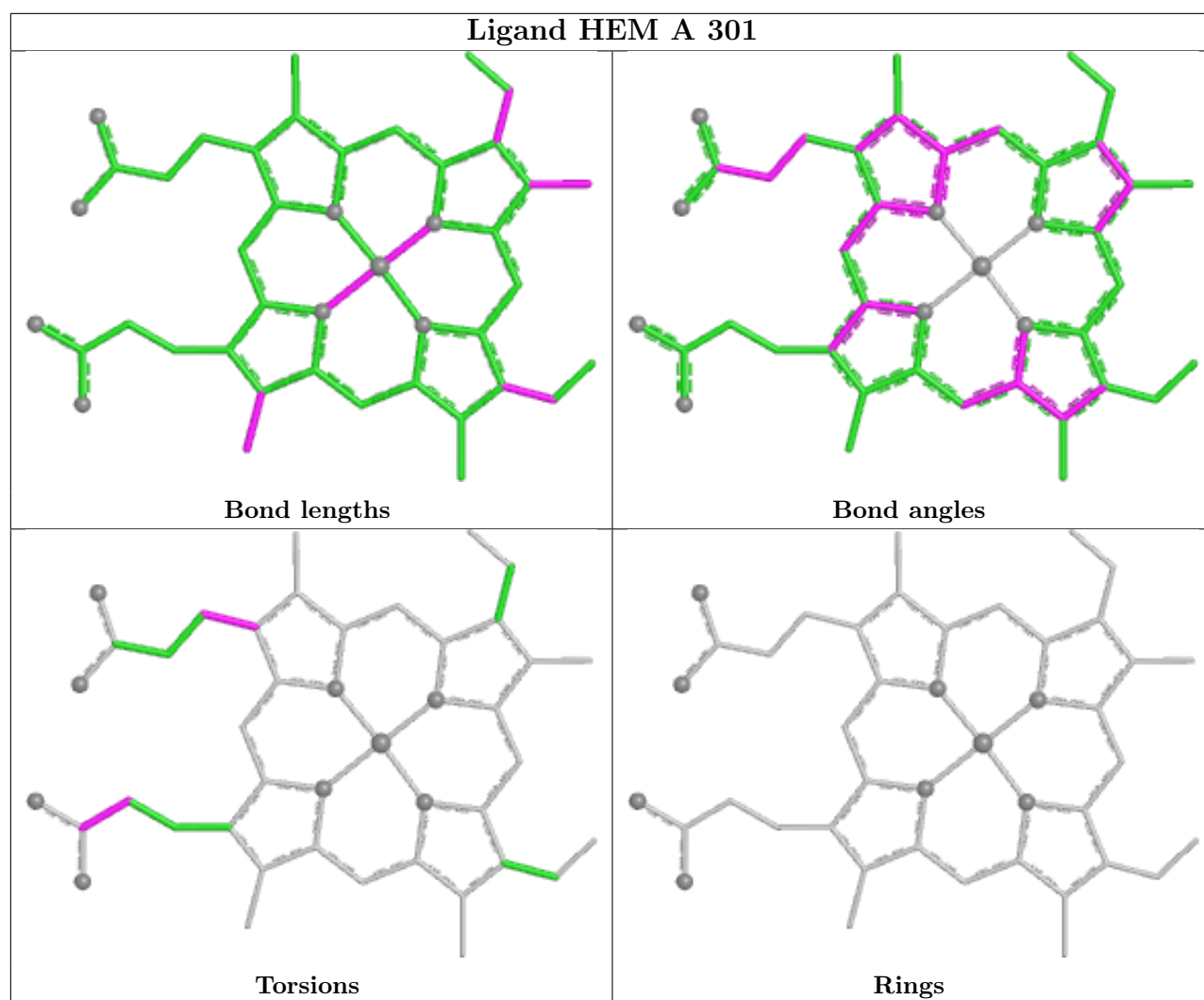
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

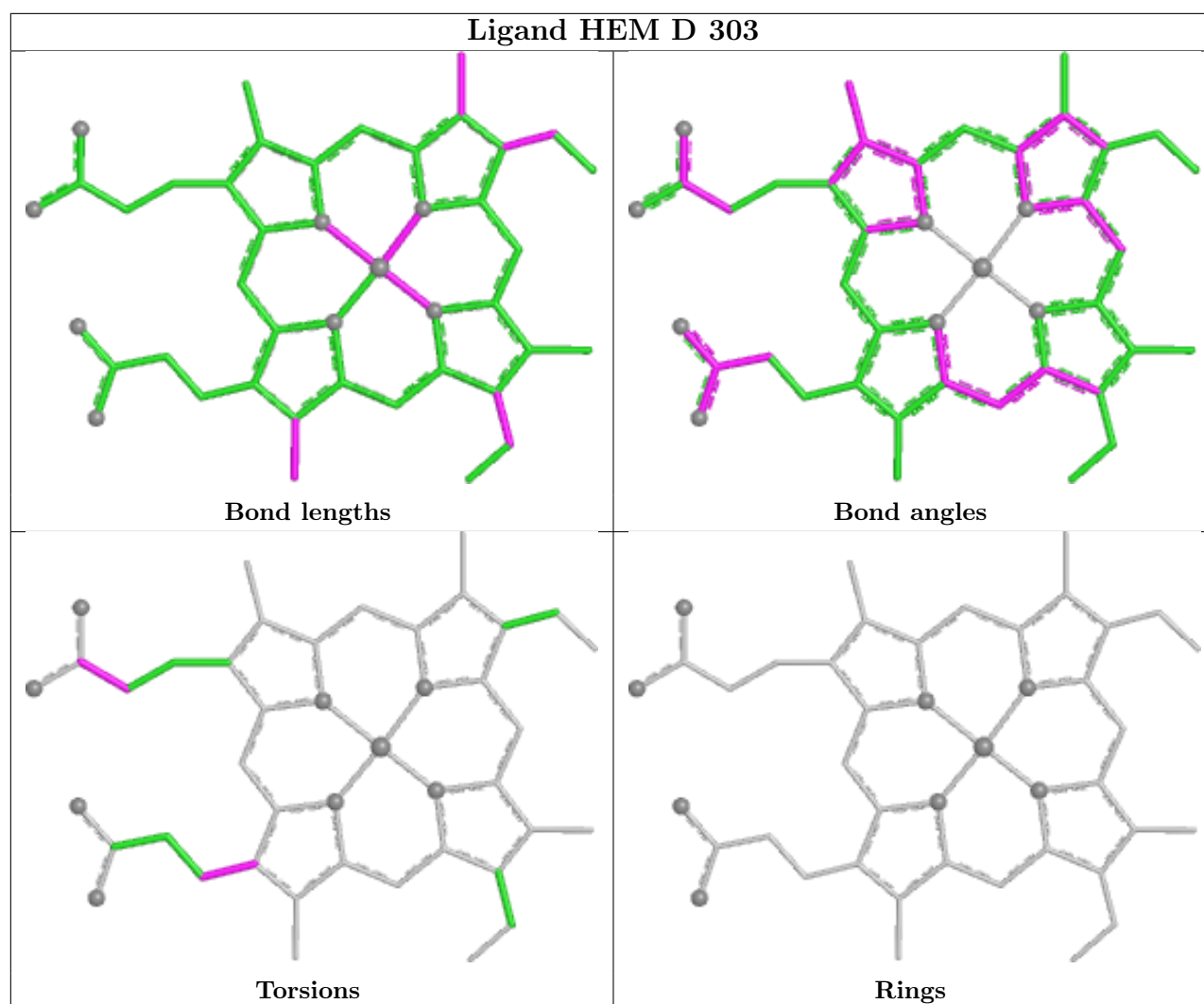












5.7 Other polymers [i](#)

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	212/229 (92%)	0.11	6 (2%)	55	59	26, 46, 91, 117	0
1	B	213/229 (93%)	0.00	6 (2%)	55	59	22, 44, 78, 100	2 (0%)
1	C	211/229 (92%)	0.03	4 (1%)	66	70	18, 42, 81, 110	1 (0%)
1	D	215/229 (93%)	0.26	13 (6%)	27	32	19, 46, 101, 132	3 (1%)
1	E	210/229 (91%)	0.22	6 (2%)	53	57	28, 46, 76, 96	0
1	F	213/229 (93%)	0.77	16 (7%)	20	23	29, 55, 98, 130	1 (0%)
All	All	1274/1374 (92%)	0.23	51 (4%)	42	48	18, 47, 91, 132	7 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	50	VAL	6.4
1	E	50	VAL	5.1
1	D	50	VAL	4.2
1	F	50	VAL	4.1
1	F	184	ARG	4.1
1	A	50	VAL	3.7
1	F	182	VAL	3.6
1	B	211	ALA	3.6
1	F	181	ALA	3.6
1	E	49	ASP	3.5
1	F	180	PRO	3.5
1	D	95	PRO	3.4
1	B	50	VAL	3.2
1	F	190	PHE	3.2
1	F	211	ALA	3.1
1	A	194	GLY	3.0
1	F	49	ASP	3.0
1	F	118	HIS	3.0
1	D	191	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	212	THR	2.9
1	D	93	LEU	2.8
1	D	211	ALA	2.8
1	A	192	ALA	2.7
1	F	151	PHE	2.6
1	C	227	HIS	2.6
1	A	49	ASP	2.6
1	E	184	ARG	2.6
1	F	183	ARG	2.6
1	D	206	ARG	2.5
1	D	49	ASP	2.5
1	F	192	ALA	2.5
1	B	49	ASP	2.4
1	C	48	THR	2.4
1	B	118	HIS	2.4
1	D	96	SER	2.4
1	F	48	THR	2.4
1	E	186	ILE	2.3
1	B	227	HIS	2.2
1	A	182	VAL	2.2
1	F	150	TYR	2.2
1	F	185	ARG	2.2
1	D	98	PRO	2.2
1	D	186	ILE	2.1
1	F	98	PRO	2.1
1	C	146	GLY	2.1
1	E	99	ALA	2.1
1	E	181	ALA	2.1
1	D	181	ALA	2.1
1	A	195	THR	2.0
1	B	194	GLY	2.0
1	D	94	TYR	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

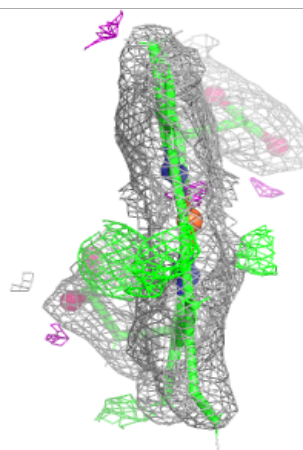
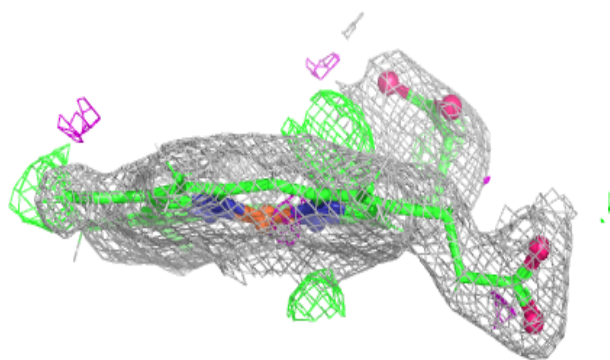
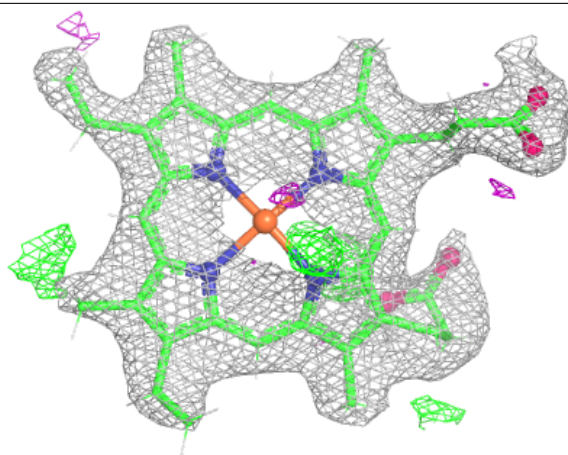
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	C	305	1/1	0.78	0.20	96,96,96,96	0
5	PEG	E	302	7/7	0.82	0.14	42,56,68,73	0
3	GOL	D	304	6/6	0.87	0.10	44,58,72,72	0
3	GOL	A	302	6/6	0.89	0.12	39,57,74,82	0
3	GOL	C	303	6/6	0.91	0.17	39,50,60,62	0
3	GOL	C	302	6/6	0.91	0.14	32,54,67,67	0
3	GOL	D	301	6/6	0.92	0.17	34,50,60,60	0
2	HEM	F	302	43/43	0.94	0.10	35,55,70,73	0
4	CA	B	303	1/1	0.95	0.11	77,77,77,77	0
2	HEM	C	301	43/43	0.97	0.08	29,45,61,72	0
2	HEM	A	301	43/43	0.98	0.06	24,35,43,50	0
2	HEM	D	303	43/43	0.98	0.06	24,34,45,54	0
2	HEM	E	301	43/43	0.98	0.06	22,34,50,55	0
2	HEM	B	302	43/43	0.98	0.06	27,41,50,53	0
4	CA	D	305	1/1	0.99	0.03	48,48,48,48	0

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

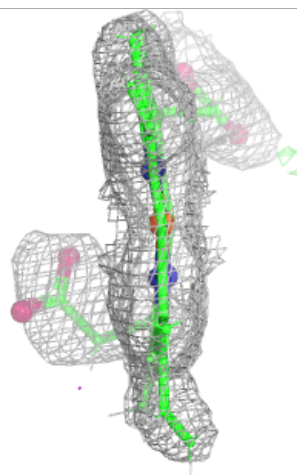
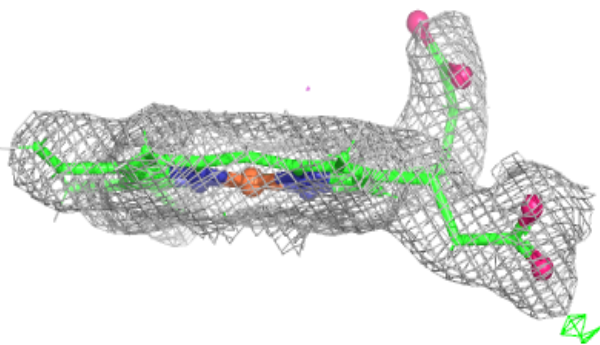
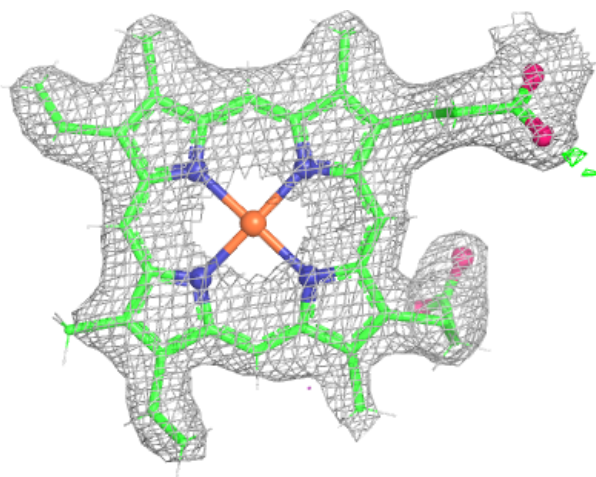
Electron density around HEM F 302:

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



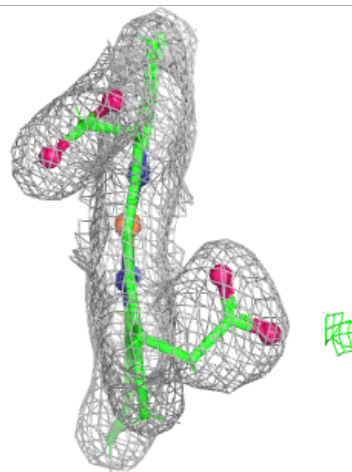
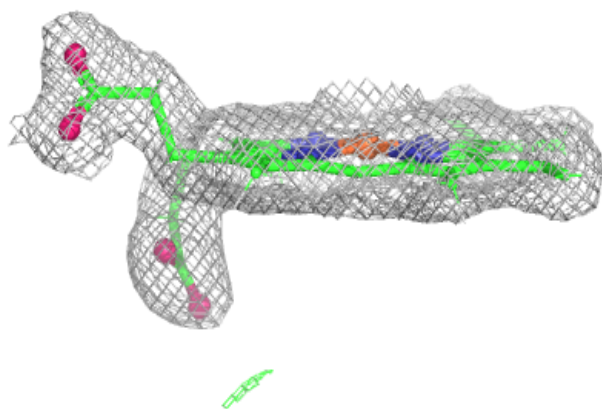
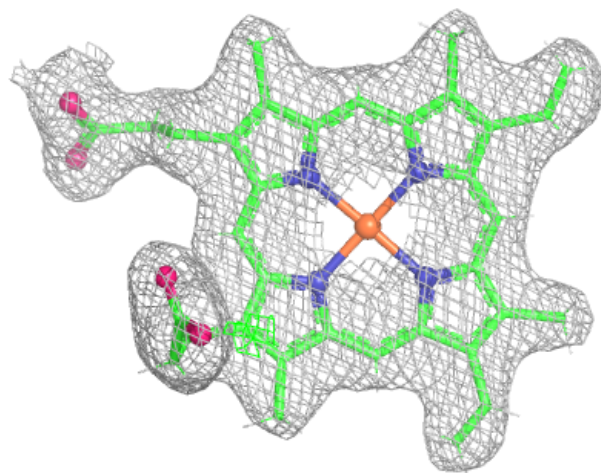
Electron density around HEM C 301:

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



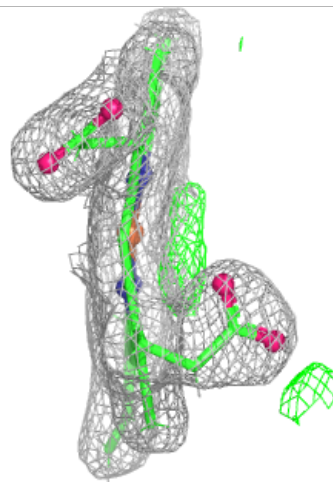
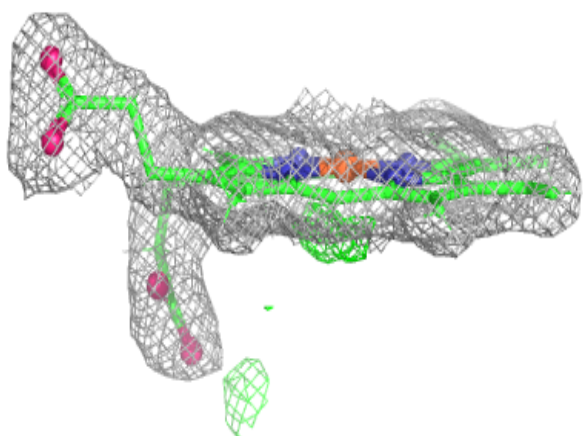
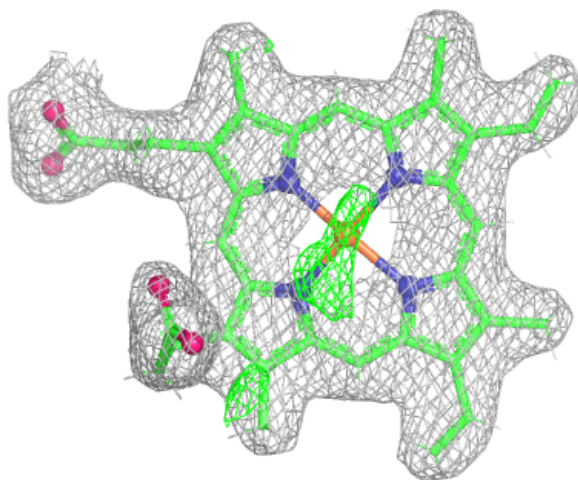
Electron density around HEM A 301:

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



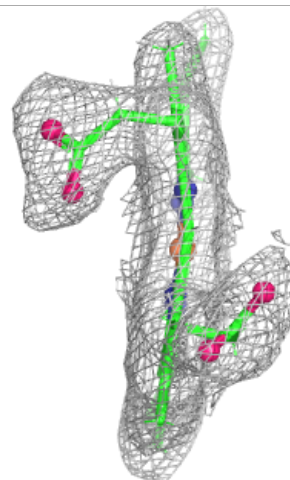
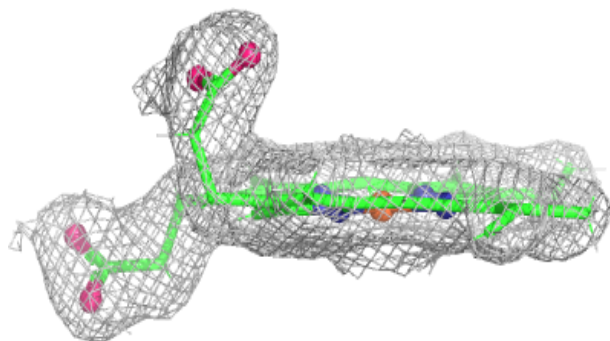
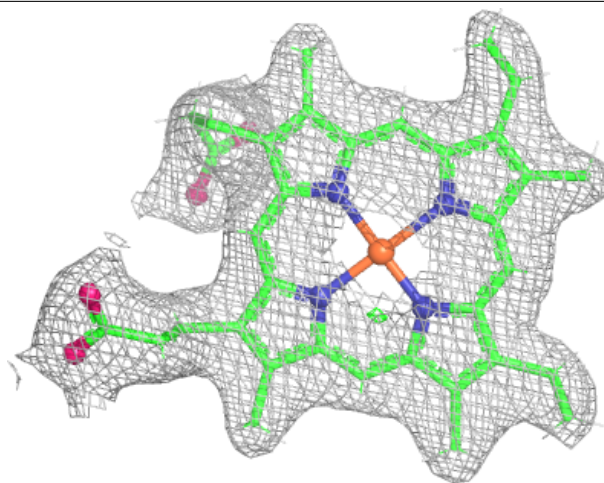
Electron density around HEM D 303:

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



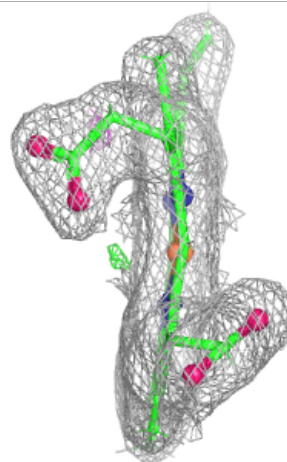
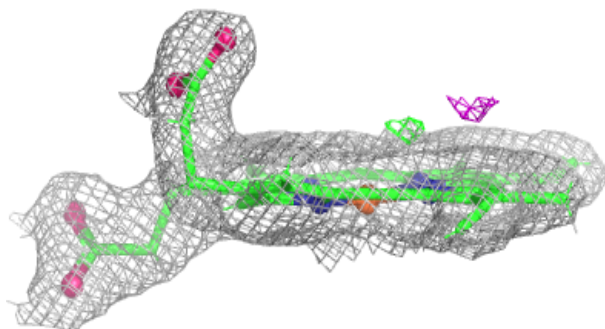
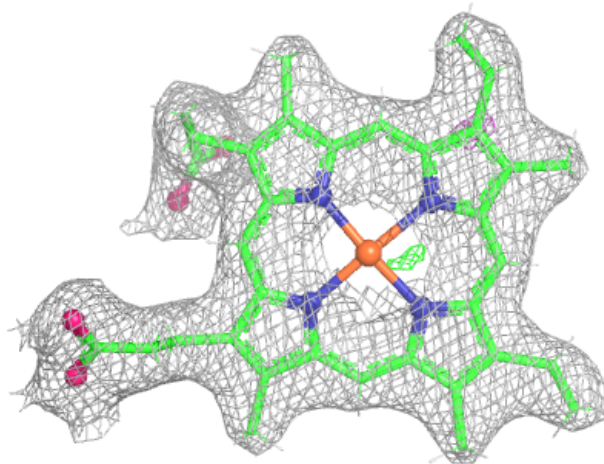
Electron density around HEM E 301:

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



Electron density around HEM B 302:

$2mF_o-DF_c$ (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.