



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 2YGX / pdb_00002ygx
Title : Structure of the mixed-function P450 MycG in P21 space group
Authors : Li, S.; Kells, P.M.; Rutaganira, F.U.; Sherman, D.H.; Podust, L.M.
Deposited on : 2011-04-22
Resolution : 2.39 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

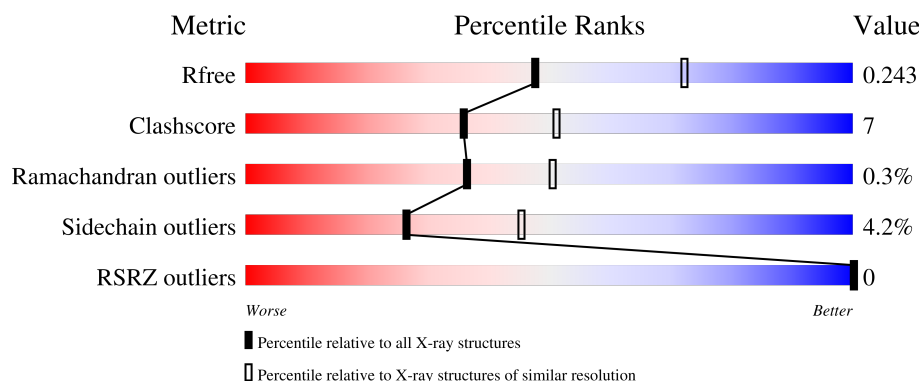
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	417	 76% 17% • 6%
1	B	417	 78% 15% • 6%
1	C	417	 76% 18% • 6%
1	D	417	 76% 17% • 6%

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	B	1401	-	-	X	-
3	GOL	C	1400	-	-	X	-
4	SIN	B	1399	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12909 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 P-450-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3056	1922	553	570	11			
1	B	393	Total	C	N	O	S	0	1	0
			3063	1926	555	571	11			
1	C	393	Total	C	N	O	S	0	0	0
			3043	1914	557	562	10			
1	D	393	Total	C	N	O	S	0	2	0
			3065	1927	558	569	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q59523
A	-18	GLY	-	expression tag	UNP Q59523
A	-17	SER	-	expression tag	UNP Q59523
A	-16	SER	-	expression tag	UNP Q59523
A	-15	HIS	-	expression tag	UNP Q59523
A	-14	HIS	-	expression tag	UNP Q59523
A	-13	HIS	-	expression tag	UNP Q59523
A	-12	HIS	-	expression tag	UNP Q59523
A	-11	HIS	-	expression tag	UNP Q59523
A	-10	HIS	-	expression tag	UNP Q59523
A	-9	SER	-	expression tag	UNP Q59523
A	-8	SER	-	expression tag	UNP Q59523
A	-7	GLY	-	expression tag	UNP Q59523
A	-6	LEU	-	expression tag	UNP Q59523
A	-5	VAL	-	expression tag	UNP Q59523
A	-4	PRO	-	expression tag	UNP Q59523
A	-3	ARG	-	expression tag	UNP Q59523
A	-2	GLY	-	expression tag	UNP Q59523
A	-1	SER	-	expression tag	UNP Q59523
A	0	HIS	-	expression tag	UNP Q59523
B	-19	MET	-	expression tag	UNP Q59523

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q59523
B	-17	SER	-	expression tag	UNP Q59523
B	-16	SER	-	expression tag	UNP Q59523
B	-15	HIS	-	expression tag	UNP Q59523
B	-14	HIS	-	expression tag	UNP Q59523
B	-13	HIS	-	expression tag	UNP Q59523
B	-12	HIS	-	expression tag	UNP Q59523
B	-11	HIS	-	expression tag	UNP Q59523
B	-10	HIS	-	expression tag	UNP Q59523
B	-9	SER	-	expression tag	UNP Q59523
B	-8	SER	-	expression tag	UNP Q59523
B	-7	GLY	-	expression tag	UNP Q59523
B	-6	LEU	-	expression tag	UNP Q59523
B	-5	VAL	-	expression tag	UNP Q59523
B	-4	PRO	-	expression tag	UNP Q59523
B	-3	ARG	-	expression tag	UNP Q59523
B	-2	GLY	-	expression tag	UNP Q59523
B	-1	SER	-	expression tag	UNP Q59523
B	0	HIS	-	expression tag	UNP Q59523
C	-19	MET	-	expression tag	UNP Q59523
C	-18	GLY	-	expression tag	UNP Q59523
C	-17	SER	-	expression tag	UNP Q59523
C	-16	SER	-	expression tag	UNP Q59523
C	-15	HIS	-	expression tag	UNP Q59523
C	-14	HIS	-	expression tag	UNP Q59523
C	-13	HIS	-	expression tag	UNP Q59523
C	-12	HIS	-	expression tag	UNP Q59523
C	-11	HIS	-	expression tag	UNP Q59523
C	-10	HIS	-	expression tag	UNP Q59523
C	-9	SER	-	expression tag	UNP Q59523
C	-8	SER	-	expression tag	UNP Q59523
C	-7	GLY	-	expression tag	UNP Q59523
C	-6	LEU	-	expression tag	UNP Q59523
C	-5	VAL	-	expression tag	UNP Q59523
C	-4	PRO	-	expression tag	UNP Q59523
C	-3	ARG	-	expression tag	UNP Q59523
C	-2	GLY	-	expression tag	UNP Q59523
C	-1	SER	-	expression tag	UNP Q59523
C	0	HIS	-	expression tag	UNP Q59523
D	-19	MET	-	expression tag	UNP Q59523
D	-18	GLY	-	expression tag	UNP Q59523
D	-17	SER	-	expression tag	UNP Q59523

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q59523
D	-15	HIS	-	expression tag	UNP Q59523
D	-14	HIS	-	expression tag	UNP Q59523
D	-13	HIS	-	expression tag	UNP Q59523
D	-12	HIS	-	expression tag	UNP Q59523
D	-11	HIS	-	expression tag	UNP Q59523
D	-10	HIS	-	expression tag	UNP Q59523
D	-9	SER	-	expression tag	UNP Q59523
D	-8	SER	-	expression tag	UNP Q59523
D	-7	GLY	-	expression tag	UNP Q59523
D	-6	LEU	-	expression tag	UNP Q59523
D	-5	VAL	-	expression tag	UNP Q59523
D	-4	PRO	-	expression tag	UNP Q59523
D	-3	ARG	-	expression tag	UNP Q59523
D	-2	GLY	-	expression tag	UNP Q59523
D	-1	SER	-	expression tag	UNP Q59523
D	0	HIS	-	expression tag	UNP Q59523

- # HEM

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

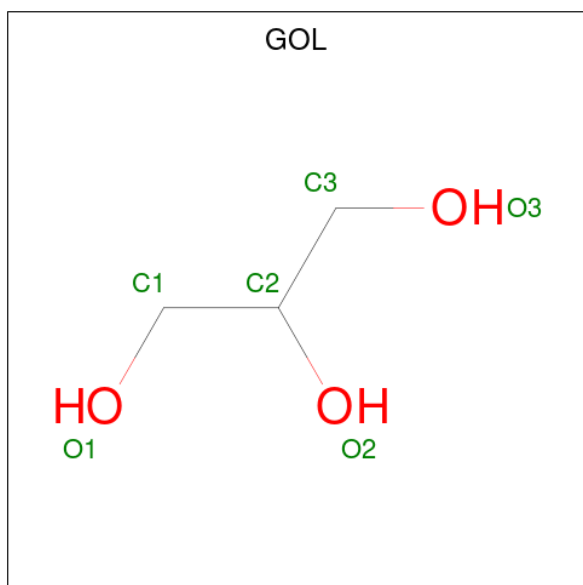


WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

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

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



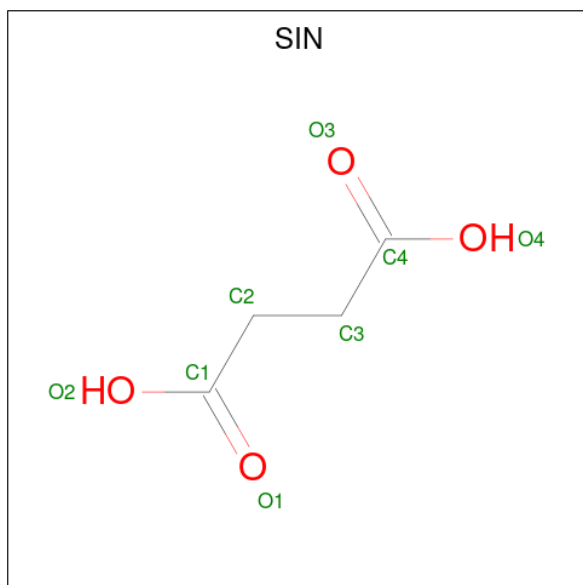
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			6	3	3		
3	A	1	Total	C	O		
			6	3	3		
3	A	1	Total	C	O		
			6	3	3		
3	A	1	Total	C	O		
			6	3	3		
3	B	1	Total	C	O		
			6	3	3		
3	B	1	Total	C	O		
			6	3	3		
3	B	1	Total	C	O		
			6	3	3		
3	C	1	Total	C	O		
			6	3	3		
3	C	1	Total	C	O		
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total	O	0	0
			113	113		
5	B	102	Total	O	0	0
			102	102		
5	C	108	Total	O	0	0
			108	108		
5	D	107	Total	O	0	0
			107	107		

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.

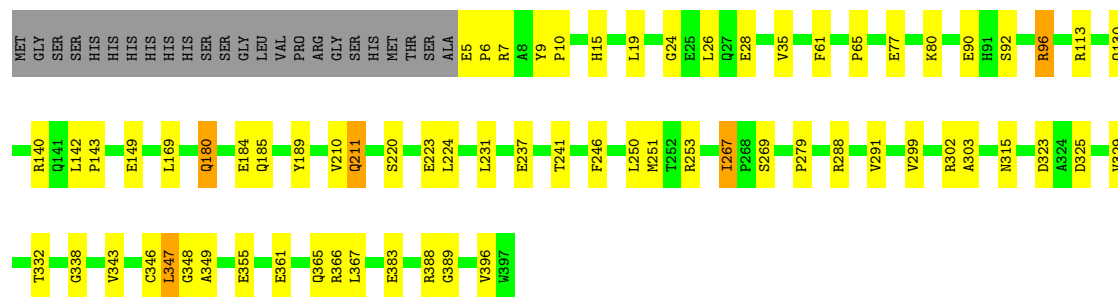
• Molecule 1: P-450-LIKE PROTEIN

Chain A: 



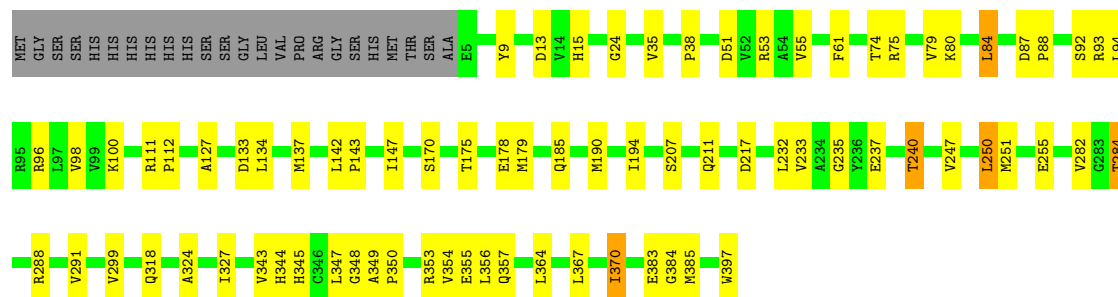
• Molecule 1: P-450-LIKE PROTEIN

Chain B: 



• Molecule 1: P-450-LIKE PROTEIN

Chain C: 



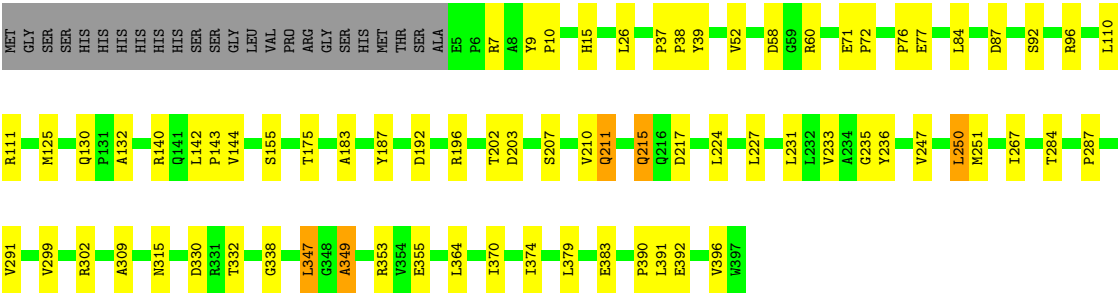
● Molecule 1: P-450-LIKE PROTEIN

Chain D:

76%

17%

• 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.15Å 161.98Å 100.11Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	80.99 – 2.39 80.99 – 2.39	Depositor EDS
% Data completeness (in resolution range)	87.4 (80.99-2.39) 87.4 (80.99-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.247 0.183 , 0.243	Depositor DCC
R_{free} test set	3191 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 7.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12909	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4580e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, HEM, SIN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.97	0/3123	1.10	7/4253 (0.2%)
1	B	1.00	1/3127 (0.0%)	1.11	7/4258 (0.2%)
1	C	1.00	0/3106	1.10	7/4231 (0.2%)
1	D	1.00	3/3130 (0.1%)	1.11	4/4263 (0.1%)
All	All	0.99	4/12486 (0.0%)	1.10	25/17005 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	ILE	CA-CB	8.72	1.59	1.54
1	D	349	ALA	CA-CB	-6.04	1.48	1.54
1	D	370	ILE	CA-CB	5.70	1.61	1.54
1	D	267	ILE	CA-CB	5.68	1.56	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	VAL	N-CA-C	-7.46	103.51	110.53
1	D	349	ALA	CA-C-N	-6.82	111.96	119.19
1	D	349	ALA	C-N-CA	-6.82	111.96	119.19
1	D	87	ASP	CA-C-N	-6.46	113.73	120.38
1	D	87	ASP	C-N-CA	-6.46	113.73	120.38
1	C	284	THR	N-CA-C	-5.97	99.97	109.59
1	A	253	ARG	CA-C-N	5.93	125.41	119.24
1	A	253	ARG	C-N-CA	5.93	125.41	119.24
1	C	87	ASP	CA-C-N	-5.89	115.42	119.66
1	C	87	ASP	C-N-CA	-5.89	115.42	119.66
1	B	349	ALA	CA-C-N	-5.78	112.63	119.05
1	B	349	ALA	C-N-CA	-5.78	112.63	119.05
1	A	53	ARG	N-CA-C	-5.76	105.08	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	VAL	N-CA-C	-5.61	105.04	110.42
1	B	253	ARG	CA-C-N	5.59	125.69	119.32
1	B	253	ARG	C-N-CA	5.59	125.69	119.32
1	B	389	GLY	CA-C-N	5.51	125.27	119.76
1	B	389	GLY	C-N-CA	5.51	125.27	119.76
1	B	251	MET	N-CA-C	-5.21	106.43	112.89
1	A	286	PHE	CA-C-N	5.20	125.12	119.76
1	A	286	PHE	C-N-CA	5.20	125.12	119.76
1	C	24	GLY	N-CA-C	-5.18	106.22	112.49
1	A	127	ALA	N-CA-C	5.09	118.26	111.75
1	C	98	VAL	N-CA-C	5.08	115.29	110.42
1	C	127	ALA	N-CA-C	5.03	118.90	112.87

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	3056	0	3022	41	0
1	B	3063	0	3032	48	0
1	C	3043	0	3019	47	0
1	D	3065	0	3021	39	0
2	A	43	0	30	3	0
2	B	43	0	30	6	0
2	C	43	0	30	4	0
2	D	43	0	30	3	0
3	A	24	0	32	6	0
3	B	18	0	24	8	0
3	C	18	0	24	8	0
3	D	12	0	16	2	0
4	B	8	0	4	0	0
5	A	113	0	0	3	0
5	B	102	0	0	0	0
5	C	108	0	0	1	0
5	D	107	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12909	0	12314	180	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 (180) 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:B:140:ARG:HH21	3:B:1401:GOL:H12	1.19	1.08
1:C:343:VAL:HG22	3:C:1398:GOL:H31	1.51	0.91
2:D:450:HEM:HBC2	2:D:450:HEM:HMC1	1.59	0.84
1:B:24:GLY:HA3	3:B:1398:GOL:H32	1.59	0.83
1:B:140:ARG:HH21	3:B:1401:GOL:C1	1.91	0.82
2:B:450:HEM:HMC1	2:B:450:HEM:HBC2	1.62	0.80
1:C:143:PRO:HA	1:C:355:GLU:OE1	1.86	0.76
1:D:52:VAL:HG13	1:D:309:ALA:HB1	1.74	0.69
1:B:113:ARG:HE	1:B:149:GLU:CD	2.02	0.67
1:C:38:PRO:HG2	1:C:74:THR:HA	1.76	0.67
1:D:96:ARG:HD3	5:D:2040:HOH:O	1.93	0.67
2:D:450:HEM:HBC2	2:D:450:HEM:CMC	2.24	0.66
1:A:327:ILE:HB	3:A:1401:GOL:H32	1.78	0.66
1:B:9:TYR:CG	1:B:10:PRO:HA	2.32	0.65
1:A:251:MET:HE1	1:A:393:LEU:HD22	1.80	0.63
1:B:241:THR:HA	3:B:1401:GOL:H32	1.79	0.63
1:D:143:PRO:HA	1:D:355:GLU:OE1	1.99	0.62
1:C:51:ASP:O	1:C:55:VAL:HG23	1.99	0.62
1:C:250:LEU:HD11	1:C:364:LEU:HD21	1.83	0.61
3:A:1398:GOL:H11	1:B:325:ASP:OD2	2.00	0.61
1:D:250:LEU:HD21	1:D:364:LEU:HD21	1.83	0.60
1:B:343:VAL:HG22	3:B:1400:GOL:C3	2.32	0.60
1:B:279:PRO:HG2	1:B:388:ARG:NH2	2.17	0.60
1:C:343:VAL:CG2	3:C:1398:GOL:H31	2.30	0.60
3:A:1401:GOL:H31	5:A:2100:HOH:O	2.01	0.60
1:C:147:ILE:HD13	1:C:232:LEU:HA	1.82	0.60
1:A:367:LEU:O	1:A:370:ILE:HG22	2.02	0.59
1:C:96:ARG:HD3	5:C:2041:HOH:O	2.01	0.58
1:D:142:LEU:HB3	1:D:143:PRO:HD3	1.84	0.57
1:C:9:TYR:HB2	1:C:35:VAL:HB	1.87	0.57
1:C:134:LEU:O	1:C:134:LEU:HG	2.03	0.57
1:C:247:VAL:HG12	1:C:251:MET:HE2	1.85	0.57
1:A:88:PRO:HB2	1:B:323:ASP:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:NH2	3:B:1401:GOL:H12	2.04	0.57
1:A:353:ARG:O	1:A:357:GLN:HG3	2.05	0.56
1:A:9:TYR:CG	1:A:10:PRO:HA	2.41	0.56
1:D:125:MET:HE2	1:D:132:ALA:HB3	1.86	0.56
1:D:9:TYR:CG	1:D:10:PRO:HA	2.41	0.56
2:B:450:HEM:HBB2	2:B:450:HEM:HMB1	1.88	0.55
1:A:147:ILE:HD13	1:A:232:LEU:HA	1.88	0.55
1:B:343:VAL:HG22	3:B:1400:GOL:H32	1.88	0.55
1:C:347:LEU:C	1:C:347:LEU:HD12	2.32	0.55
1:D:58:ASP:OD1	1:D:60:ARG:HB2	2.06	0.55
1:C:175:THR:OG1	1:C:178:GLU:HG3	2.07	0.55
1:C:349:ALA:O	1:C:353:ARG:HG3	2.07	0.55
1:A:135:VAL:HG23	1:A:393:LEU:HB2	1.87	0.55
1:A:143:PRO:HA	1:A:355:GLU:OE1	2.06	0.54
1:D:71:GLU:OE2	1:D:287:PRO:HG2	2.08	0.53
1:A:240:THR:HG22	3:A:1400:GOL:H12	1.91	0.53
1:B:130:GLN:HB3	1:B:396:VAL:HG12	1.90	0.53
1:C:240:THR:HG22	3:C:1399:GOL:H32	1.90	0.53
1:C:350:PRO:O	1:C:354:VAL:HG23	2.09	0.53
1:D:183:ALA:O	1:D:187:TYR:HD1	1.91	0.53
1:B:366:ARG:O	1:B:367:LEU:HD23	2.09	0.52
1:D:9:TYR:CD1	1:D:10:PRO:HA	2.43	0.52
1:A:175:THR:OG1	1:A:178:GLU:HB2	2.10	0.52
1:D:207:SER:O	1:D:211:GLN:HG2	2.09	0.52
1:A:5:GLU:N	1:A:6:PRO:HD2	2.24	0.51
1:B:269:SER:OG	1:B:329:VAL:O	2.27	0.51
1:C:61:PHE:HB3	1:C:288:ARG:HB3	1.92	0.51
1:A:347:LEU:C	1:A:347:LEU:HD12	2.36	0.51
1:B:220:SER:OG	1:B:223:GLU:HG3	2.10	0.51
1:C:207:SER:O	1:C:211:GLN:HG2	2.11	0.51
1:A:250:LEU:HD22	1:A:364:LEU:HD21	1.93	0.51
1:C:15:HIS:HE1	1:C:383:GLU:OE2	1.94	0.50
2:B:450:HEM:HBC2	2:B:450:HEM:CMC	2.37	0.50
1:B:7:ARG:CZ	1:B:26:LEU:HD21	2.42	0.50
3:A:1398:GOL:C1	1:B:325:ASP:OD2	2.60	0.49
1:C:367:LEU:O	1:C:370:ILE:HG22	2.12	0.49
1:B:15:HIS:HE1	1:B:383:GLU:OE2	1.94	0.49
1:C:348:GLY:HA3	2:C:450:HEM:C3C	2.48	0.49
1:D:349:ALA:O	1:D:353:ARG:HG3	2.12	0.49
1:A:134:LEU:HG	1:A:134:LEU:O	2.12	0.49
1:A:9:TYR:HB2	1:A:35:VAL:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:GLY:O	1:C:385:MET:HB2	2.13	0.49
1:A:250:LEU:CD1	1:A:360:LEU:HD22	2.42	0.49
1:C:255:GLU:HB2	3:C:1400:GOL:H32	1.95	0.49
1:C:318:GLN:HE22	1:C:324:ALA:H	1.61	0.48
1:B:347:LEU:C	1:B:347:LEU:HD12	2.38	0.48
1:C:142:LEU:HB3	1:C:143:PRO:HD3	1.94	0.48
1:C:190:MET:O	1:C:194:ILE:HD12	2.13	0.48
1:C:327:ILE:HB	3:C:1400:GOL:H12	1.96	0.48
1:C:353:ARG:O	1:C:357:GLN:HG3	2.13	0.48
1:D:39:TYR:CZ	1:D:76:PRO:HG3	2.48	0.48
1:A:78:MET:HB2	5:A:2037:HOH:O	2.14	0.48
1:D:390:PRO:O	3:D:1398:GOL:H32	2.13	0.48
1:C:13:ASP:OD1	1:C:15:HIS:HD2	1.98	0.47
1:B:142:LEU:HB3	1:B:143:PRO:HD3	1.96	0.47
1:A:207:SER:O	1:A:211:GLN:HG2	2.14	0.47
1:C:133:ASP:O	1:C:137:MET:HG3	2.15	0.47
1:C:255:GLU:HB2	3:C:1400:GOL:C3	2.44	0.47
1:C:327:ILE:O	3:C:1400:GOL:H12	2.14	0.47
1:D:302:ARG:HG2	1:D:302:ARG:HH11	1.79	0.47
1:D:140:ARG:HH21	3:D:1398:GOL:H31	1.78	0.47
1:A:288:ARG:O	1:A:307:VAL:N	2.48	0.47
1:C:318:GLN:NE2	1:C:324:ALA:H	2.13	0.47
1:D:247:VAL:O	1:D:251:MET:HG3	2.14	0.46
1:B:9:TYR:CD1	1:B:10:PRO:HA	2.50	0.46
1:B:113:ARG:HG2	1:B:113:ARG:HH11	1.80	0.46
1:C:13:ASP:OD1	1:C:15:HIS:CD2	2.69	0.46
1:B:5:GLU:HB3	1:B:6:PRO:HD3	1.97	0.46
1:B:169:LEU:HD22	1:B:237:GLU:HG3	1.98	0.46
1:D:215:GLN:C	1:D:217:ASP:H	2.23	0.46
1:B:9:TYR:HB2	1:B:35:VAL:HB	1.97	0.46
1:C:75:ARG:HD2	1:C:384:GLY:O	2.16	0.46
1:D:9:TYR:O	1:D:38:PRO:HD3	2.15	0.46
1:A:84:LEU:HD22	2:A:450:HEM:HAD2	1.97	0.45
1:A:284:THR:OG1	1:A:308:LEU:HB3	2.16	0.45
1:A:96:ARG:HD3	5:A:2050:HOH:O	2.15	0.45
1:B:90:GLU:H	1:B:90:GLU:CD	2.25	0.45
1:D:211:GLN:HE21	1:D:211:GLN:HB3	1.53	0.45
1:B:92:SER:O	1:B:96:ARG:HB2	2.17	0.45
1:D:37:PRO:HG3	1:D:72:PRO:HB3	1.99	0.45
1:B:143:PRO:HA	1:B:355:GLU:OE1	2.17	0.45
1:A:7:ARG:NH1	1:A:26:LEU:HD21	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:HIS:HE1	1:A:383:GLU:OE2	2.00	0.44
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.77	0.44
1:B:343:VAL:HG22	3:B:1400:GOL:H31	1.97	0.44
1:B:361:GLU:O	1:B:365:GLN:HB2	2.17	0.44
1:B:61:PHE:HB3	1:B:288:ARG:HB3	1.99	0.44
1:B:246:PHE:O	1:B:250:LEU:HD23	2.17	0.44
1:D:210:VAL:HG22	1:D:224:LEU:HD13	1.99	0.44
1:D:347:LEU:HD12	1:D:347:LEU:C	2.43	0.44
1:A:386:LEU:O	1:A:387:LEU:HD23	2.16	0.44
1:D:7:ARG:CZ	1:D:26:LEU:HD21	2.47	0.44
1:D:227:LEU:O	1:D:231:LEU:HG	2.17	0.44
1:A:367:LEU:HD22	1:A:397:TRP:CG	2.52	0.44
1:B:279:PRO:HG2	1:B:388:ARG:HH22	1.81	0.44
1:B:302:ARG:HH11	1:B:302:ARG:HG2	1.83	0.44
1:B:346:CYS:HB2	2:B:450:HEM:NA	2.33	0.43
1:C:88:PRO:HB3	1:C:92:SER:OG	2.17	0.43
1:A:133:ASP:O	1:A:137:MET:HG3	2.19	0.43
1:C:93:ARG:NE	1:C:217:ASP:OD2	2.43	0.43
1:D:235:GLY:HA2	2:D:450:HEM:C2C	2.54	0.43
1:A:95:ARG:O	1:A:99:VAL:HG22	2.17	0.43
1:D:130:GLN:HB3	1:D:396:VAL:HG12	2.01	0.43
1:D:192[B]:ASP:O	1:D:196:ARG:HG3	2.19	0.43
1:C:92:SER:O	1:C:96:ARG:HB2	2.19	0.43
1:C:240:THR:HG22	3:C:1399:GOL:C3	2.48	0.43
1:D:144:VAL:HB	1:D:236:TYR:CE1	2.54	0.43
1:A:276:ARG:O	1:A:315:ASN:HB3	2.19	0.43
1:A:75:ARG:HD3	1:A:384:GLY:O	2.19	0.43
1:B:189:TYR:CD1	1:B:189:TYR:C	2.97	0.43
1:B:211:GLN:HE21	1:B:211:GLN:HB3	1.46	0.42
1:B:210:VAL:HG22	1:B:224:LEU:HD13	2.00	0.42
1:D:92:SER:O	1:D:96:ARG:HB2	2.19	0.42
1:B:348:GLY:HA3	2:B:450:HEM:C3C	2.54	0.42
1:C:344:HIS:O	1:C:345:HIS:C	2.61	0.42
1:B:15:HIS:CE1	1:B:383:GLU:OE2	2.73	0.42
1:A:250:LEU:CD2	1:A:364:LEU:HD21	2.50	0.42
1:A:16:GLY:HA2	1:A:381:TRP:CZ2	2.53	0.42
1:D:110:LEU:O	1:D:111:ARG:C	2.59	0.42
1:A:61:PHE:HB3	1:A:288:ARG:HB3	2.01	0.42
1:D:315:ASN:HD21	1:D:338:GLY:N	2.18	0.42
1:B:180:GLN:NE2	1:B:184:GLU:OE2	2.50	0.42
1:A:253:ARG:HD3	3:A:1401:GOL:O3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:SER:OG	1:C:237:GLU:OE2	2.33	0.42
1:C:235:GLY:HA2	2:C:450:HEM:C2C	2.54	0.42
1:D:125:MET:HE2	1:D:132:ALA:CB	2.50	0.42
1:B:9:TYR:CD2	1:B:10:PRO:HA	2.55	0.41
1:C:9:TYR:O	1:C:38:PRO:HD3	2.20	0.41
1:C:356:LEU:HD11	2:C:450:HEM:HBB1	2.02	0.41
1:C:367:LEU:HD22	1:C:397:TRP:CG	2.55	0.41
1:A:155:SER:C	1:A:157:ASP:N	2.77	0.41
1:A:99:VAL:HG21	1:B:28:GLU:HG3	2.03	0.41
1:A:235:GLY:HA2	2:A:450:HEM:C2C	2.55	0.41
1:B:315:ASN:HD21	1:B:338:GLY:N	2.19	0.41
2:B:450:HEM:HBB2	2:B:450:HEM:CMB	2.51	0.41
1:D:391:LEU:HD23	1:D:391:LEU:HA	1.85	0.41
1:B:19:LEU:HA	1:B:19:LEU:HD12	1.83	0.41
1:D:202:THR:HB	1:D:203:ASP:H	1.60	0.41
1:A:181:GLU:O	1:A:185:GLN:HG2	2.21	0.41
1:D:374:ILE:HD11	1:D:379:LEU:HD23	2.03	0.41
1:A:348:GLY:HA3	2:A:450:HEM:C3C	2.56	0.41
1:B:302:ARG:O	1:B:303:ALA:C	2.62	0.40
1:C:111:ARG:HB3	1:C:112:PRO:HD3	2.03	0.40
1:D:15:HIS:HE1	1:D:383:GLU:OE2	2.04	0.40
1:C:84:LEU:HD13	2:C:450:HEM:O1D	2.20	0.40
1:D:9:TYR:OH	1:D:284:THR:HG23	2.21	0.40
1:A:278:VAL:HA	1:A:279:PRO:HD3	1.99	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	392/417 (94%)	373 (95%)	16 (4%)	3 (1%)	16 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	392/417 (94%)	376 (96%)	16 (4%)	0	100	100
1	C	391/417 (94%)	372 (95%)	19 (5%)	0	100	100
1	D	393/417 (94%)	378 (96%)	14 (4%)	1 (0%)	36	50
All	All	1568/1668 (94%)	1499 (96%)	65 (4%)	4 (0%)	36	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	215	GLN
1	A	215	GLN
1	A	285	ALA
1	A	76	PRO

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	317/346 (92%)	304 (96%)	13 (4%)	27	46
1	B	318/346 (92%)	306 (96%)	12 (4%)	29	49
1	C	314/346 (91%)	299 (95%)	15 (5%)	23	40
1	D	316/346 (91%)	303 (96%)	13 (4%)	27	46
All	All	1265/1384 (91%)	1212 (96%)	53 (4%)	26	45

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	79	VAL
1	A	80	LYS
1	A	84	LEU
1	A	162	THR
1	A	178	GLU
1	A	233	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	LEU
1	A	255	GLU
1	A	291	VAL
1	A	299	VAL
1	A	332	THR
1	A	347	LEU
1	B	65	PRO
1	B	77	GLU
1	B	80	LYS
1	B	96	ARG
1	B	180	GLN
1	B	185	GLN
1	B	211	GLN
1	B	267	ILE
1	B	291	VAL
1	B	299	VAL
1	B	332	THR
1	B	347	LEU
1	C	53	ARG
1	C	79	VAL
1	C	80	LYS
1	C	84	LEU
1	C	94	LEU
1	C	100	LYS
1	C	179	MET
1	C	185	GLN
1	C	233	VAL
1	C	240	THR
1	C	250	LEU
1	C	284	THR
1	C	291	VAL
1	C	299	VAL
1	C	370	ILE
1	D	77	GLU
1	D	84	LEU
1	D	155	SER
1	D	175	THR
1	D	211	GLN
1	D	233	VAL
1	D	250	LEU
1	D	291	VAL
1	D	299	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	330	ASP
1	D	332	THR
1	D	347	LEU
1	D	392	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	130	GLN
1	A	211	GLN
1	A	259	GLN
1	A	318	GLN
1	B	15	HIS
1	B	130	GLN
1	B	211	GLN
1	B	259	GLN
1	B	318	GLN
1	B	335	GLN
1	C	15	HIS
1	C	130	GLN
1	C	211	GLN
1	C	318	GLN
1	C	320	GLN
1	C	335	GLN
1	C	365	GLN
1	C	378	GLN
1	D	15	HIS
1	D	130	GLN
1	D	180	GLN
1	D	211	GLN
1	D	259	GLN
1	D	318	GLN

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](#)

17 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	450	1,5	50,50,50	1.90	8 (16%)	67,82,82	1.35	7 (10%)
3	GOL	B	1401	-	5,5,5	0.53	0	5,5,5	1.21	0
3	GOL	C	1400	-	5,5,5	0.34	0	5,5,5	1.28	0
2	HEM	A	450	1,5	50,50,50	1.79	10 (20%)	67,82,82	1.21	7 (10%)
3	GOL	D	1398	-	5,5,5	0.37	0	5,5,5	1.08	1 (20%)
3	GOL	A	1399	-	5,5,5	0.26	0	5,5,5	0.72	0
3	GOL	A	1401	-	5,5,5	0.52	0	5,5,5	1.46	1 (20%)
2	HEM	D	450	1	50,50,50	1.86	10 (20%)	67,82,82	1.48	11 (16%)
3	GOL	B	1398	-	5,5,5	0.58	0	5,5,5	0.90	0
3	GOL	D	1399	-	5,5,5	0.51	0	5,5,5	1.03	0
2	HEM	B	450	1	50,50,50	1.91	8 (16%)	67,82,82	1.46	11 (16%)
3	GOL	A	1400	-	5,5,5	0.42	0	5,5,5	0.38	0
3	GOL	C	1398	-	5,5,5	0.30	0	5,5,5	0.92	0
3	GOL	B	1400	-	5,5,5	0.49	0	5,5,5	0.54	0
3	GOL	A	1398	-	5,5,5	0.38	0	5,5,5	0.93	0
4	SIN	B	1399	-	7,7,7	1.20	0	8,8,8	1.89	4 (50%)
3	GOL	C	1399	-	5,5,5	0.32	0	5,5,5	1.08	0

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	450	1,5	-	2/14/54/54	-
3	GOL	B	1401	-	-	0/4/4/4	-
3	GOL	C	1400	-	-	2/4/4/4	-
2	HEM	A	450	1,5	-	0/14/54/54	-
3	GOL	D	1398	-	-	3/4/4/4	-
3	GOL	A	1399	-	-	0/4/4/4	-
3	GOL	A	1401	-	-	2/4/4/4	-
2	HEM	D	450	1	-	0/14/54/54	-
3	GOL	B	1398	-	-	2/4/4/4	-
3	GOL	D	1399	-	-	2/4/4/4	-
2	HEM	B	450	1	-	0/14/54/54	-
3	GOL	A	1400	-	-	3/4/4/4	-
3	GOL	C	1398	-	-	3/4/4/4	-
3	GOL	B	1400	-	-	4/4/4/4	-
3	GOL	A	1398	-	-	2/4/4/4	-
4	SIN	B	1399	-	-	5/5/5/5	-
3	GOL	C	1399	-	-	2/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	450	HEM	C3D-C2D	7.67	1.53	1.36
2	A	450	HEM	C3D-C2D	7.46	1.52	1.36
2	D	450	HEM	C3D-C2D	6.90	1.51	1.36
2	B	450	HEM	C3D-C2D	6.73	1.51	1.36
2	D	450	HEM	FE-NA	5.84	2.14	1.95
2	B	450	HEM	FE-ND	5.55	2.12	1.94
2	B	450	HEM	FE-NA	5.15	2.12	1.95
2	C	450	HEM	FE-ND	4.96	2.10	1.94
2	C	450	HEM	FE-NC	4.27	2.09	1.95
2	A	450	HEM	FE-ND	3.86	2.06	1.94
2	C	450	HEM	FE-NB	3.86	2.06	1.94
2	A	450	HEM	FE-NC	3.82	2.07	1.95
2	C	450	HEM	CAC-C3C	3.11	1.55	1.47
2	A	450	HEM	CAC-C3C	3.08	1.55	1.47
2	B	450	HEM	FE-NB	3.03	2.04	1.94
2	D	450	HEM	CMC-C2C	2.95	1.56	1.50
2	B	450	HEM	CAC-C3C	2.73	1.54	1.47
2	B	450	HEM	CMC-C2C	2.71	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	450	HEM	CMB-C2B	2.71	1.56	1.50
2	D	450	HEM	FE-NB	2.71	2.03	1.94
2	D	450	HEM	CAB-C3B	2.65	1.54	1.47
2	A	450	HEM	FE-NA	2.61	2.03	1.95
2	B	450	HEM	CAB-C3B	2.55	1.54	1.47
2	A	450	HEM	CMC-C2C	2.53	1.56	1.50
2	D	450	HEM	C3C-C4C	-2.34	1.41	1.46
2	C	450	HEM	CMD-C2D	2.26	1.55	1.50
2	D	450	HEM	CAC-C3C	2.23	1.53	1.47
2	A	450	HEM	C2A-C3A	-2.22	1.33	1.38
2	D	450	HEM	C2A-C3A	-2.13	1.33	1.38
2	A	450	HEM	CMB-C2B	2.13	1.55	1.50
2	A	450	HEM	C3B-C2B	-2.09	1.32	1.37
2	B	450	HEM	FE-NC	2.07	2.02	1.95
2	A	450	HEM	CAB-C3B	2.03	1.52	1.47
2	C	450	HEM	O1A-CGA	2.03	1.28	1.22
2	D	450	HEM	CMD-C2D	2.03	1.54	1.50
2	C	450	HEM	FE-NA	2.00	2.01	1.95

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	450	HEM	C4D-ND-C1D	4.63	110.69	105.21
2	C	450	HEM	C3B-C4B-NB	-4.32	106.36	109.47
2	A	450	HEM	C4D-ND-C1D	4.17	110.14	105.21
2	B	450	HEM	CMD-C2D-C1D	4.01	131.29	125.03
2	B	450	HEM	C3B-C4B-NB	-3.95	106.63	109.47
2	B	450	HEM	C4D-ND-C1D	3.94	109.87	105.21
2	D	450	HEM	CHD-C4C-NC	3.87	128.66	124.45
2	D	450	HEM	CMD-C2D-C1D	3.70	130.81	125.03
2	D	450	HEM	C4C-C3C-C2C	3.69	110.02	106.81
2	D	450	HEM	C4D-ND-C1D	3.67	109.55	105.21
2	B	450	HEM	C1B-NB-C4B	3.38	109.21	105.21
2	D	450	HEM	CHA-C4D-ND	3.38	128.55	124.37
2	A	450	HEM	C3B-C4B-NB	-2.86	107.41	109.47
4	B	1399	SIN	O2-C1-C2	2.76	122.72	114.00
4	B	1399	SIN	O4-C4-O3	-2.75	116.27	123.33
2	A	450	HEM	C4B-C3B-C2B	2.70	109.76	107.28
2	C	450	HEM	C1B-NB-C4B	2.68	108.39	105.21
2	B	450	HEM	CHC-C4B-NB	2.57	127.19	124.42
2	D	450	HEM	C4B-C3B-C2B	2.52	109.60	107.28
2	C	450	HEM	C4B-C3B-C2B	2.50	109.57	107.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1399	SIN	O4-C4-C3	2.48	121.83	114.00
4	B	1399	SIN	O2-C1-O1	-2.44	117.06	123.33
3	A	1401	GOL	O2-C2-C3	2.41	119.17	109.18
2	B	450	HEM	CHD-C4C-NC	2.31	126.96	124.45
2	C	450	HEM	CHC-C4B-NB	2.30	126.89	124.42
2	C	450	HEM	CAD-C3D-C4D	2.30	128.70	124.70
2	B	450	HEM	CHA-C4D-ND	2.29	127.20	124.37
2	B	450	HEM	CAD-C3D-C4D	2.27	128.65	124.70
2	D	450	HEM	C1D-C2D-C3D	-2.26	104.60	106.98
2	A	450	HEM	O2D-CGD-CBD	2.26	121.13	114.00
2	C	450	HEM	C1D-C2D-C3D	-2.25	104.61	106.98
2	A	450	HEM	CHC-C4B-NB	2.23	126.82	124.42
2	D	450	HEM	CAC-C3C-C4C	-2.21	119.55	124.82
2	B	450	HEM	C1D-C2D-C3D	-2.17	104.70	106.98
2	A	450	HEM	CBD-CAD-C3D	-2.13	106.65	112.53
2	A	450	HEM	CAD-C3D-C4D	2.11	128.38	124.70
2	B	450	HEM	C3A-C4A-NA	-2.11	106.76	110.14
2	B	450	HEM	C4A-C3A-C2A	2.09	109.21	106.82
2	D	450	HEM	CBD-CAD-C3D	-2.08	106.78	112.53
3	D	1398	GOL	O3-C3-C2	-2.07	101.05	110.38
2	D	450	HEM	CBC-CAC-C3C	-2.07	117.20	127.53
2	D	450	HEM	C3B-C4B-NB	-2.05	108.00	109.47

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1398	GOL	O1-C1-C2-C3
3	A	1401	GOL	O1-C1-C2-C3
3	B	1398	GOL	O1-C1-C2-C3
3	B	1400	GOL	O1-C1-C2-O2
3	B	1400	GOL	O1-C1-C2-C3
3	B	1400	GOL	C1-C2-C3-O3
3	C	1398	GOL	C1-C2-C3-O3
3	C	1400	GOL	C1-C2-C3-O3
3	C	1400	GOL	O2-C2-C3-O3
3	D	1399	GOL	C1-C2-C3-O3
4	B	1399	SIN	C1-C2-C3-C4
3	C	1399	GOL	O1-C1-C2-O2
3	A	1400	GOL	C1-C2-C3-O3
3	A	1401	GOL	C1-C2-C3-O3
3	C	1399	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1398	GOL	O1-C1-C2-C3
3	B	1398	GOL	O1-C1-C2-O2
3	B	1400	GOL	O2-C2-C3-O3
3	C	1398	GOL	O2-C2-C3-O3
3	D	1399	GOL	O2-C2-C3-O3
2	C	450	HEM	C2B-C3B-CAB-CBB
2	C	450	HEM	C4B-C3B-CAB-CBB
3	A	1398	GOL	O1-C1-C2-O2
3	A	1400	GOL	O1-C1-C2-C3
3	D	1398	GOL	C1-C2-C3-O3
3	D	1398	GOL	O1-C1-C2-O2
4	B	1399	SIN	C2-C3-C4-O4
4	B	1399	SIN	C2-C3-C4-O3
3	C	1398	GOL	O1-C1-C2-O2
3	A	1400	GOL	O2-C2-C3-O3
4	B	1399	SIN	O1-C1-C2-C3
4	B	1399	SIN	O2-C1-C2-C3

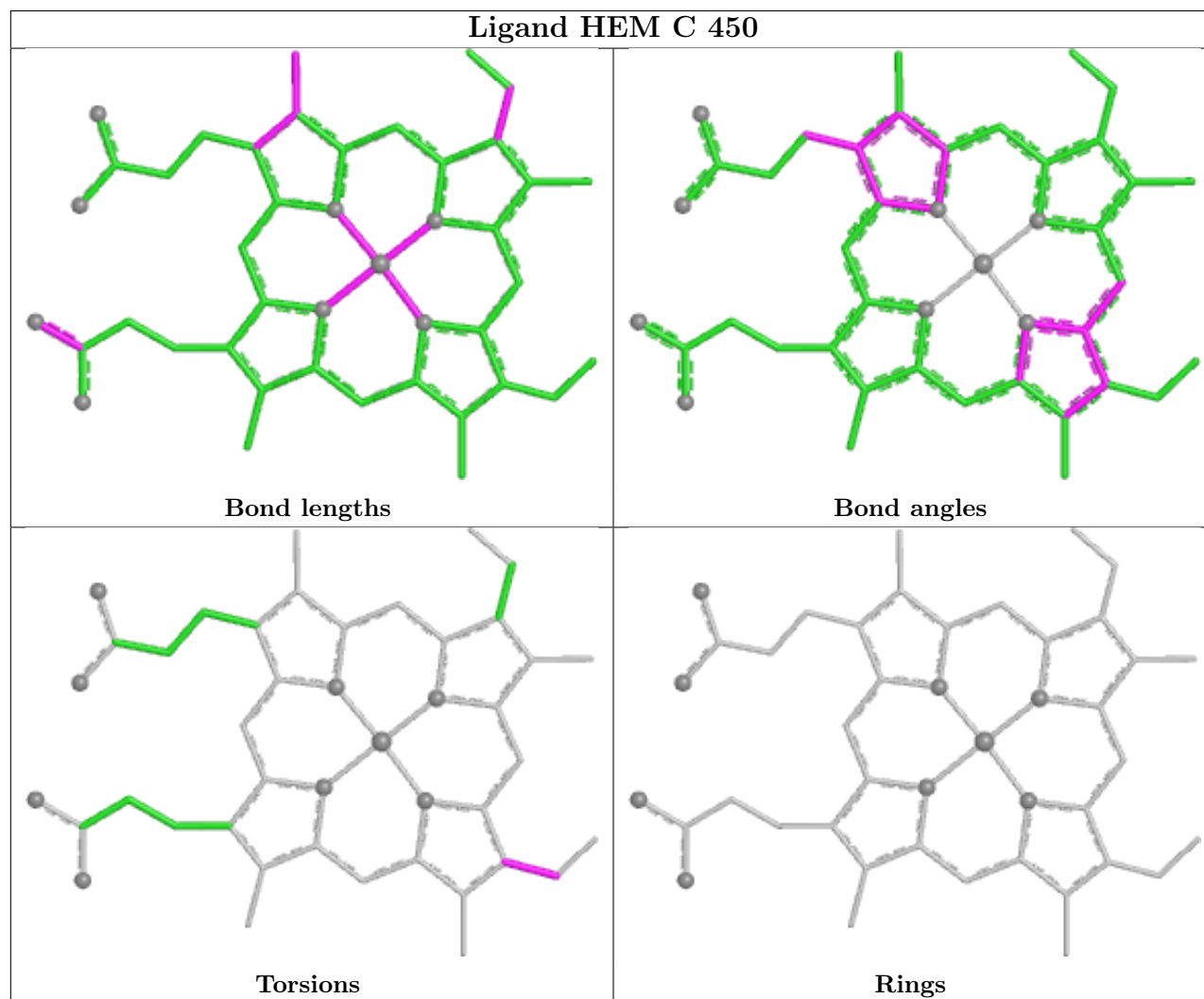
There are no ring outliers.

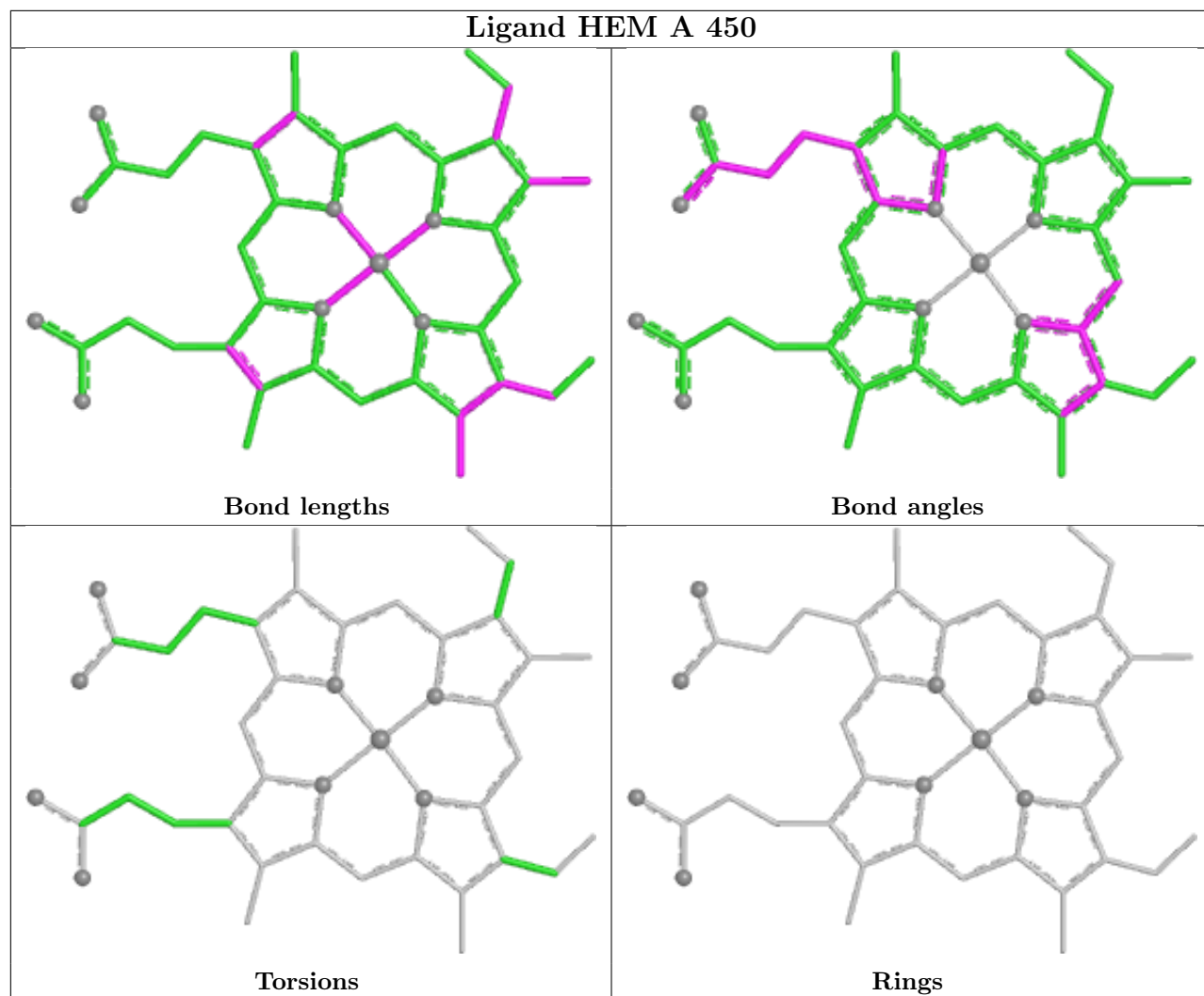
14 monomers are involved in 40 short contacts:

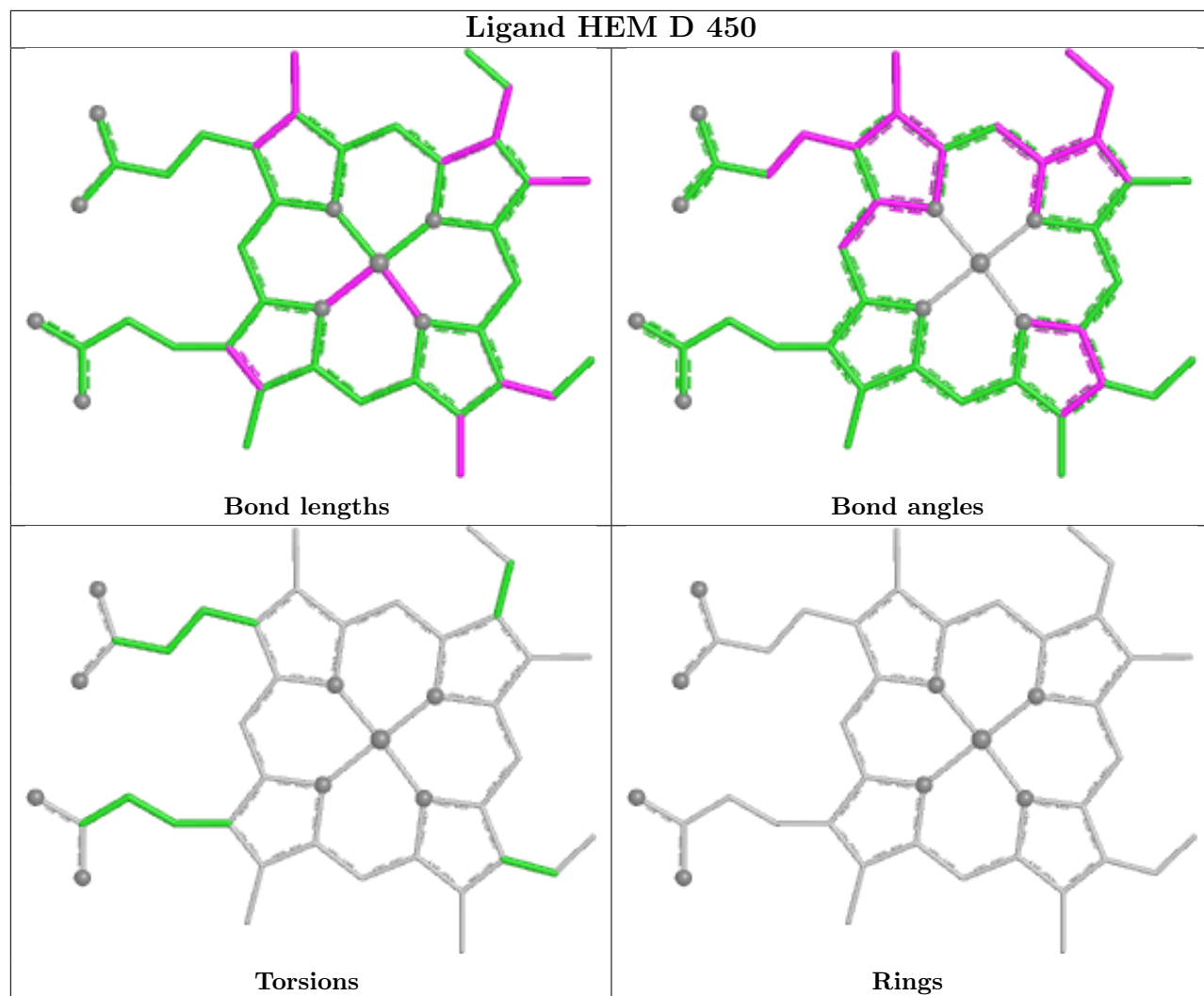
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	450	HEM	4	0
3	B	1401	GOL	4	0
3	C	1400	GOL	4	0
2	A	450	HEM	3	0
3	D	1398	GOL	2	0
3	A	1401	GOL	3	0
2	D	450	HEM	3	0
3	B	1398	GOL	1	0
2	B	450	HEM	6	0
3	A	1400	GOL	1	0
3	C	1398	GOL	2	0
3	B	1400	GOL	3	0
3	A	1398	GOL	2	0
3	C	1399	GOL	2	0

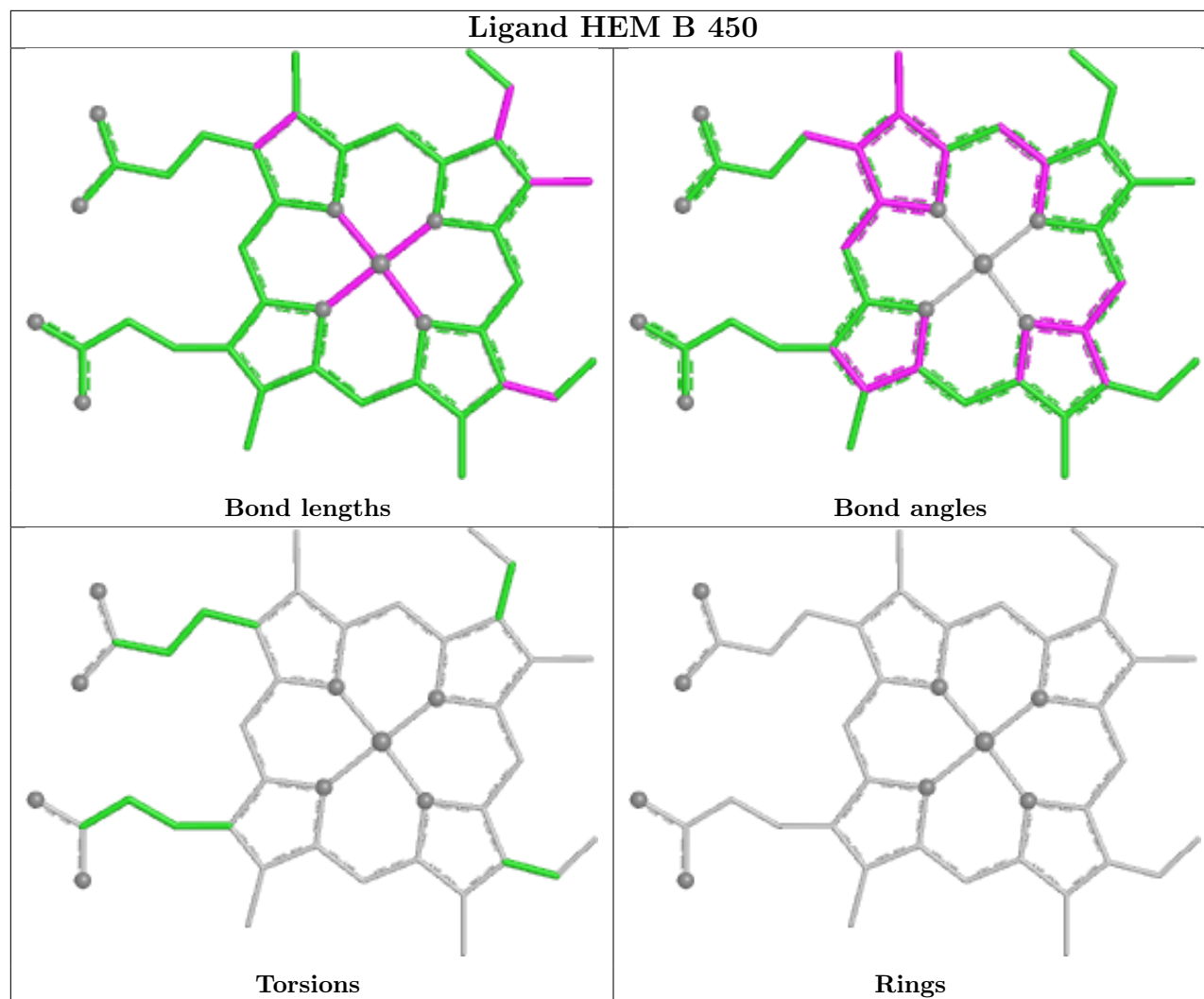
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/417 (94%)	-2.10	0 100 100	8, 21, 37, 54	1 (0%)
1	B	393/417 (94%)	-2.11	0 100 100	7, 20, 37, 56	1 (0%)
1	C	393/417 (94%)	-2.10	0 100 100	9, 21, 37, 51	0
1	D	393/417 (94%)	-2.10	0 100 100	6, 20, 37, 50	2 (0%)
All	All	1572/1668 (94%)	-2.10	0 100 100	6, 20, 37, 56	4 (0%)

There are no RSRZ outliers to report.

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
2	HEM	A	450	43/43	1.00	0.01	5,11,14,17	0
2	HEM	B	450	43/43	1.00	0.01	2,10,14,19	0
2	HEM	C	450	43/43	1.00	0.01	2,10,14,16	0
2	HEM	D	450	43/43	1.00	0.01	4,9,14,15	0

Continued on next page...

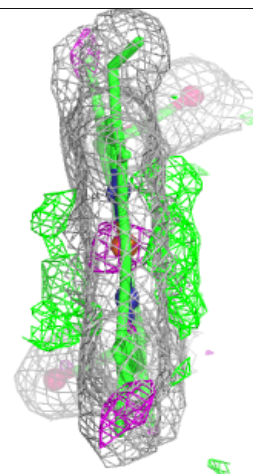
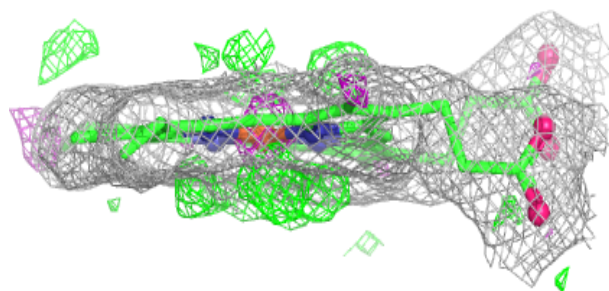
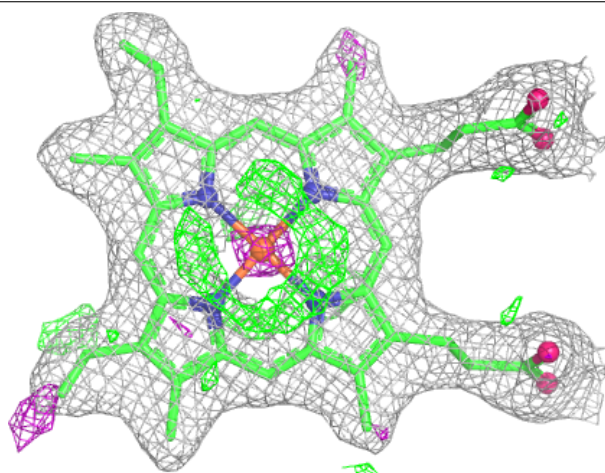
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1398	6/6	1.00	0.01	12,18,19,20	0
3	GOL	A	1399	6/6	1.00	0.01	36,38,40,43	0
3	GOL	A	1400	6/6	1.00	0.01	22,26,27,28	0
3	GOL	A	1401	6/6	1.00	0.01	30,36,38,40	0
3	GOL	B	1398	6/6	1.00	0.01	48,51,52,52	0
3	GOL	B	1400	6/6	1.00	0.01	10,21,23,25	0
3	GOL	B	1401	6/6	1.00	0.01	25,30,32,35	0
3	GOL	C	1398	6/6	1.00	0.01	14,15,18,24	0
3	GOL	C	1399	6/6	1.00	0.01	20,22,23,24	0
3	GOL	C	1400	6/6	1.00	0.01	32,35,38,39	0
3	GOL	D	1398	6/6	1.00	0.01	23,28,29,29	0
3	GOL	D	1399	6/6	1.00	0.01	12,19,20,24	0
4	SIN	B	1399	8/8	1.00	0.02	69,70,74,75	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.

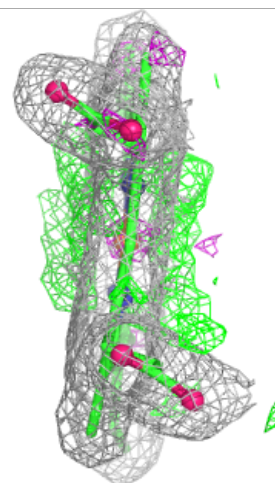
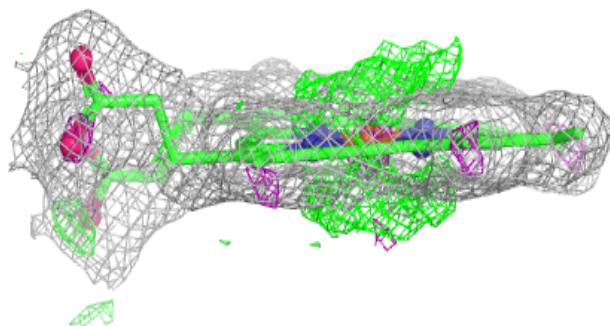
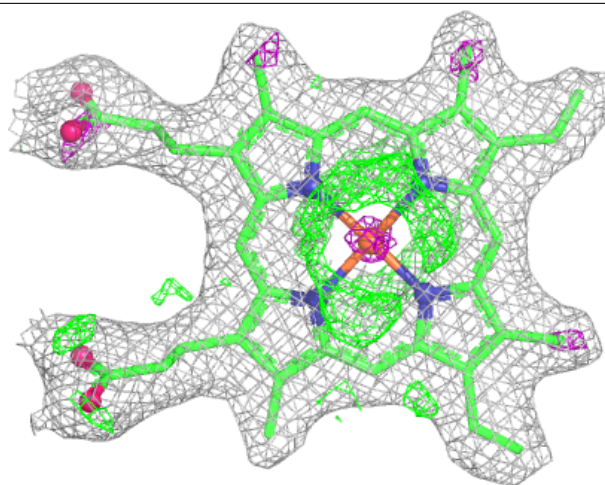
Electron density around HEM A 450:

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



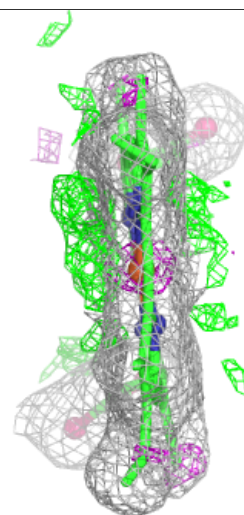
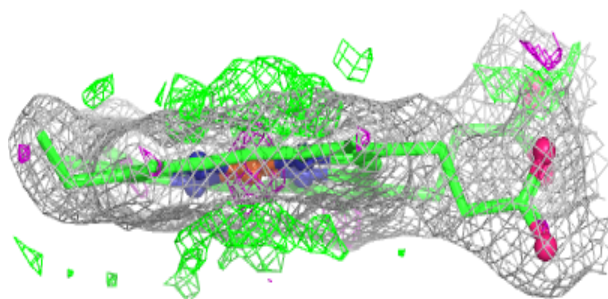
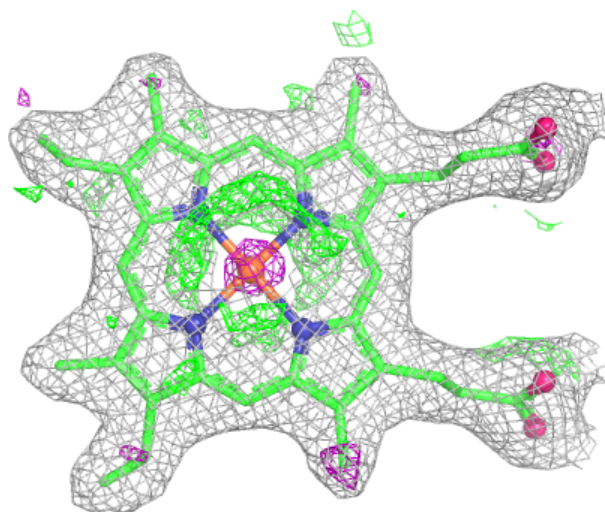
Electron density around HEM B 450:

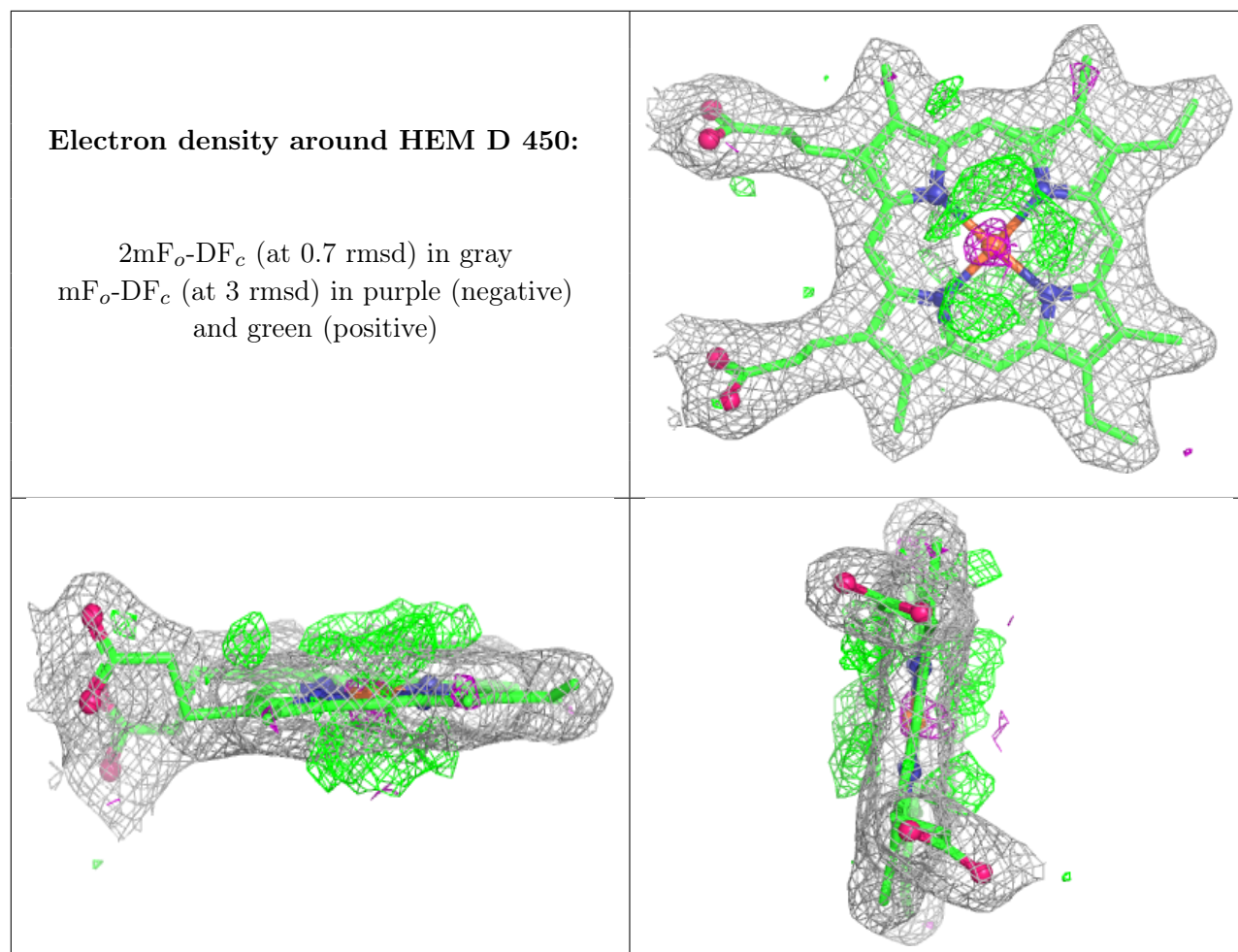
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 450:

$2mF_o-DF_c$ (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.