



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:46 PM JST

PDB ID : 6L8H / pdb_00006l8h
Title : Crystal structure of CYP97C1
Authors : Niu, G.; Guo, Q.; Liu, L.
Deposited on : 2019-11-06
Resolution : 2.00 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

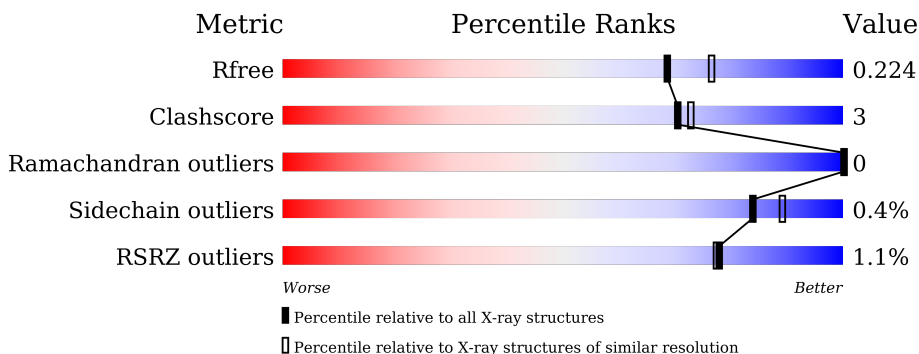
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	471	92% 7% .
1	B	471	2% 91% 8% .
1	C	471	% 89% 9% .
1	D	471	% 93% 6% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16945 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.

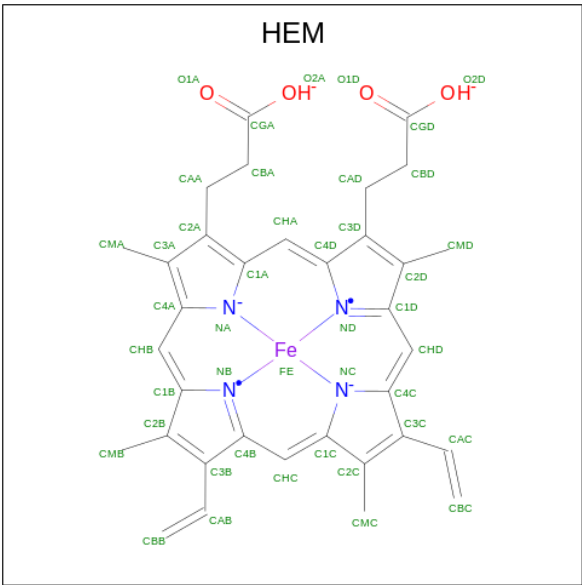
- Molecule 1 is a protein called Carotene epsilon-monooxygenase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	10	0
			3722	2380	637	690	15			
1	B	465	Total	C	N	O	S	0	5	0
			3663	2343	622	683	15			
1	C	465	Total	C	N	O	S	0	6	0
			3684	2357	625	687	15			
1	D	466	Total	C	N	O	S	0	3	0
			3660	2341	623	681	15			

There are 4 discrepancies between the modelled and reference sequences:

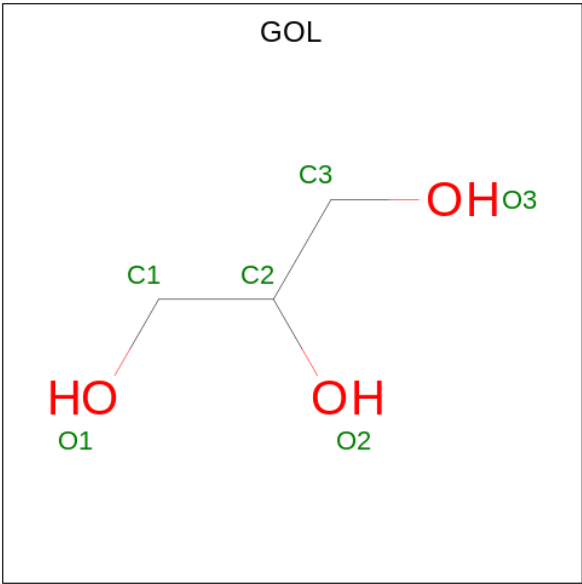
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	-	expression tag	UNP Q6TBX7
B	69	GLY	-	expression tag	UNP Q6TBX7
C	69	GLY	-	expression tag	UNP Q6TBX7
D	69	GLY	-	expression tag	UNP Q6TBX7

- 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).



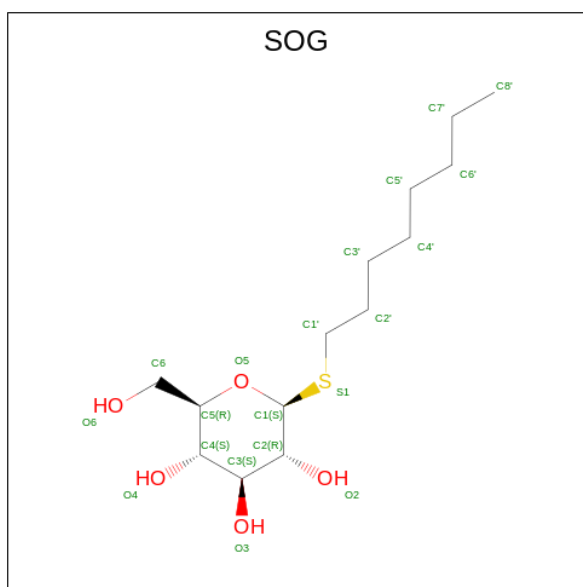
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 4 is octyl 1-thio-beta-D-glucopyranoside (CCD ID: SOG) (formula: $C_{14}H_{28}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			20	14	5	1		
4	B	1	Total	C	O	S	0	0
			20	14	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	S	0	0
			20	14	5	1		
4	D	1	Total	C	O	S	0	0
			20	14	5	1		

- Molecule 5 is water.

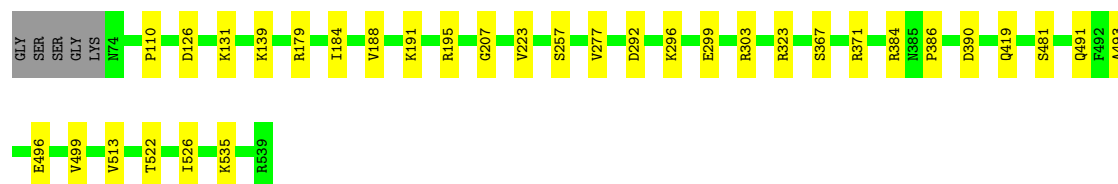
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	652	Total	O	0	0
			652	652		
5	B	414	Total	O	0	0
			414	414		
5	C	446	Total	O	0	0
			446	446		
5	D	392	Total	O	0	0
			392	392		

3 Residue-property plots [i](#)

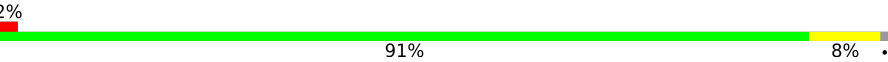
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

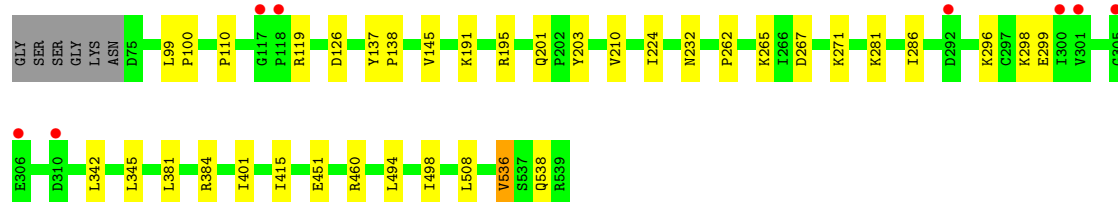
- Molecule 1: Carotene epsilon-monooxygenase, chloroplactic

Chain A: 



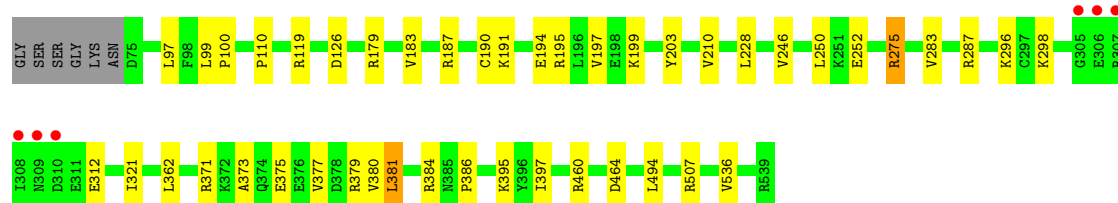
- Molecule 1: Carotene epsilon-monooxygenase, chloroplactic

Chain B: 

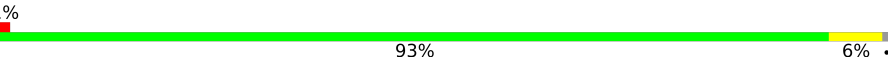


- Molecule 1: Carotene epsilon-monooxygenase, chloroplactic

Chain C: 



- Molecule 1: Carotene epsilon-monooxygenase, chloroplactic

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.75Å 127.32Å 143.67Å 90.00° 92.22° 90.00°	Depositor
Resolution (Å)	40.70 – 2.00 40.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.2 (40.70-2.00) 89.7 (40.70-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.172 , 0.224 0.173 , 0.224	Depositor DCC
R_{free} test set	6850 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16945	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/3823	0.54	0/5188
1	B	0.31	0/3752	0.48	0/5098
1	C	0.36	2/3776 (0.1%)	0.48	0/5127
1	D	0.29	0/3743	0.47	0/5084
All	All	0.34	2/15094 (0.0%)	0.49	0/20497

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	371	ARG	C-O	-6.76	1.16	1.24
1	C	460	ARG	C-O	-5.29	1.17	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3722	0	3767	23	0
1	B	3663	0	3675	23	0
1	C	3684	0	3715	31	0
1	D	3660	0	3675	19	0
2	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	2	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	12	0	16	1	0
3	B	12	0	16	0	0
3	C	18	0	24	1	0
3	D	18	0	24	0	0
4	A	20	0	28	1	0
4	B	20	0	28	4	0
4	C	20	0	28	2	0
4	D	20	0	28	2	0
5	A	652	0	0	8	0
5	B	414	0	0	3	0
5	C	446	0	0	5	0
5	D	392	0	0	4	0
All	All	16945	0	15144	102	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 3.

All (102) 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:145:VAL:HG22	4:B:604:SOG:H62	1.68	0.75
1:C:191:LYS:HE2	1:C:195:ARG:HH22	1.51	0.74
1:B:401:ILE:HD12	1:B:498:ILE:HD13	1.73	0.71
1:A:131:LYS:NZ	5:A:702:HOH:O	2.27	0.67
1:B:451:GLU:O	1:B:460:ARG:NH2	2.27	0.66
1:B:298:LYS:NZ	5:B:703:HOH:O	2.29	0.65
1:D:287:ARG:NH1	5:D:709:HOH:O	2.30	0.65
1:A:257:SER:HB2	4:A:604:SOG:H4	1.78	0.64
1:C:296:LYS:NZ	5:C:704:HOH:O	2.28	0.63
1:B:119:ARG:HG3	4:B:604:SOG:H7'1	1.82	0.62
1:B:262:PRO:HB2	1:B:265:LYS:HD2	1.82	0.62
1:C:179:ARG:NH1	1:C:312:GLU:O	2.33	0.61
1:C:199:LYS:NZ	5:C:707:HOH:O	2.32	0.61
1:A:323:ARG:NH2	5:A:710:HOH:O	2.33	0.60
1:B:281:LYS:NZ	5:B:710:HOH:O	2.35	0.60
1:B:494:LEU:O	1:B:498:ILE:HG12	2.03	0.59
1:B:381:LEU:O	1:B:384:ARG:HG2	2.02	0.58
1:C:97:LEU:HD13	4:C:605:SOG:H2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HE2	1:A:195:ARG:HH22	1.68	0.57
1:C:252:GLU:OE1	1:C:275:ARG:HD2	2.04	0.57
1:C:110:PRO:HB2	1:C:126:ASP:HB2	1.86	0.57
1:C:381:LEU:O	1:C:384:ARG:HG2	2.05	0.57
1:C:312:GLU:N	5:C:715:HOH:O	2.38	0.56
1:B:99:LEU:HB3	1:B:100:PRO:HD3	1.89	0.55
1:B:296:LYS:O	1:B:299:GLU:HG2	2.07	0.53
1:A:386:PRO:HG2	1:A:499:VAL:HG13	1.90	0.53
1:C:373:ALA:O	1:C:377[B]:VAL:HG13	2.09	0.53
1:D:110:PRO:HB2	1:D:126:ASP:HB2	1.91	0.53
1:B:267:ASP:OD1	1:B:271:LYS:NZ	2.42	0.53
1:B:201:GLN:OE1	1:B:538:GLN:NE2	2.37	0.52
1:B:191:LYS:HE3	1:B:195:ARG:HH22	1.74	0.52
1:A:110:PRO:HB2	1:A:126:ASP:HB2	1.93	0.51
1:C:377[B]:VAL:HG12	1:C:397:ILE:HD11	1.93	0.51
1:A:419[A]:GLN:NE2	5:A:703:HOH:O	2.27	0.50
1:C:99:LEU:HB3	1:C:100:PRO:HD3	1.92	0.50
1:A:522:THR:HG22	1:A:526:ILE:HG12	1.94	0.49
1:B:145:VAL:HG23	1:B:415:ILE:HB	1.93	0.49
1:C:380:VAL:HG12	1:C:381:LEU:HD13	1.95	0.49
1:A:491[B]:GLN:NE2	5:A:722:HOH:O	2.44	0.49
1:A:179:ARG:NH2	5:A:729:HOH:O	2.46	0.48
1:C:246:VAL:O	1:C:250:LEU:HG	2.14	0.48
1:C:377[B]:VAL:CG1	1:C:397:ILE:HD11	2.43	0.47
1:A:384[A]:ARG:NH2	1:A:390:ASP:OD2	2.43	0.47
1:D:99:LEU:HB3	1:D:100:PRO:HD3	1.96	0.47
1:C:298:LYS:HE3	1:C:298:LYS:HB2	1.75	0.46
1:D:191:LYS:HE2	1:D:195:ARG:HH22	1.79	0.46
1:A:139:LYS:HE2	5:A:807:HOH:O	2.16	0.46
1:C:228:LEU:HD23	1:C:321:ILE:HD12	1.97	0.46
1:B:203:TYR:CD1	1:B:210:VAL:HB	2.51	0.46
1:D:480:PHE:HB3	1:D:487:CYS:HB3	1.97	0.46
2:B:601:HEM:O1A	5:B:701:HOH:O	2.21	0.46
1:A:481:SER:CB	2:A:601:HEM:HAA1	2.47	0.45
1:D:306:GLU:OE2	1:D:313:TYR:OH	2.27	0.45
1:B:119:ARG:CG	4:B:604:SOG:H7'1	2.46	0.45
1:C:190:CYS:SG	1:C:386:PRO:HD2	2.56	0.45
1:C:197:VAL:HG11	1:C:507:ARG:HD2	1.97	0.45
1:B:508:LEU:HD22	1:B:536:VAL:HG13	1.98	0.45
1:A:367:SER:O	1:A:371:ARG:HG2	2.16	0.45
1:A:207:GLY:O	1:A:535:LYS:HE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:OE2	1:A:303:ARG:NH1	2.50	0.44
1:D:183:VAL:HG21	1:D:314:VAL:HG11	1.99	0.44
1:A:481:SER:HB2	2:A:601:HEM:HAA1	1.99	0.44
1:C:395:LYS:NZ	1:C:464[B]:ASP:OD1	2.42	0.44
1:C:203:TYR:CD1	1:C:210:VAL:HB	2.53	0.44
1:C:119:ARG:HH11	1:C:119:ARG:HG3	1.83	0.43
1:D:389:GLU:HG3	5:D:1012:HOH:O	2.17	0.43
1:A:513:VAL:HG22	1:A:535:LYS:HD3	2.00	0.43
1:A:195:ARG:NE	5:A:750:HOH:O	2.51	0.43
1:A:292[A]:ASP:OD1	1:A:296:LYS:NZ	2.52	0.43
1:C:494:LEU:HD23	1:C:494:LEU:HA	1.91	0.43
1:B:110:PRO:HB2	1:B:126:ASP:HB2	2.01	0.43
1:C:97:LEU:O	1:C:100:PRO:HD2	2.19	0.43
1:C:362:LEU:HD21	3:C:603:GOL:H11	2.00	0.43
1:A:493:ALA:HB2	2:A:601:HEM:HHC	2.00	0.42
4:B:604:SOG:H6'1	4:B:604:SOG:H3'1	1.75	0.42
4:D:605:SOG:H5'2	4:D:605:SOG:H2'1	1.23	0.42
1:B:137:TYR:CD1	1:B:138:PRO:HA	2.55	0.42
1:C:183:VAL:HG13	1:C:187:ARG:HD3	2.01	0.42
1:C:373:ALA:O	1:C:377[A]:VAL:HG23	2.20	0.42
1:D:503:VAL:HA	1:D:506:GLN:HG2	2.02	0.42
1:B:224:ILE:HG23	1:B:345:LEU:HD12	2.01	0.42
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	2.02	0.42
1:D:191:LYS:CE	1:D:195:ARG:HH22	2.33	0.42
1:C:377[A]:VAL:CG2	1:C:397:ILE:HD11	2.48	0.42
1:D:139:LYS:HE2	5:D:720:HOH:O	2.20	0.42
1:D:145:VAL:HG23	1:D:415:ILE:HB	2.02	0.42
1:C:375[A]:GLU:CD	1:C:379:ARG:HH21	2.28	0.41
1:D:191:LYS:NZ	1:D:195:ARG:HH22	2.18	0.41
1:B:286:ILE:CG2	1:B:342:LEU:HD11	2.49	0.41
1:B:195:ARG:NH1	1:B:232:ASN:HD21	2.19	0.41
1:D:297:CYS:SG	1:D:323:ARG:HD3	2.60	0.41
1:A:223:VAL:HG11	1:A:496:GLU:CD	2.46	0.41
3:A:602:GOL:H32	5:A:1125:HOH:O	2.19	0.41
1:D:116:ALA:HB3	4:D:605:SOG:H8'1	2.03	0.41
4:C:605:SOG:H3	5:C:971:HOH:O	2.21	0.41
1:D:260:LEU:HD23	1:D:260:LEU:HA	1.67	0.41
1:C:283:VAL:HG12	1:C:287:ARG:HD2	2.03	0.41
1:D:211:ASN:HB2	1:D:533:TYR:CE2	2.56	0.41
1:D:441:TYR:CZ	1:D:445:ARG:HD2	2.56	0.41
1:A:184:ILE:HG23	1:A:188:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLU:OE1	5:C:701:HOH:O	2.21	0.40
1:D:371[A]:ARG:HG3	5:D:886:HOH:O	2.21	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	474/471 (101%)	469 (99%)	5 (1%)	0	100	100
1	B	468/471 (99%)	462 (99%)	6 (1%)	0	100	100
1	C	469/471 (100%)	462 (98%)	7 (2%)	0	100	100
1	D	467/471 (99%)	458 (98%)	9 (2%)	0	100	100
All	All	1878/1884 (100%)	1851 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	406/407 (100%)	405 (100%)	1 (0%)	87	92
1	B	396/407 (97%)	395 (100%)	1 (0%)	86	91
1	C	401/407 (98%)	398 (99%)	3 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	395/407 (97%)	394 (100%)	1 (0%)	86	91
All	All	1598/1628 (98%)	1592 (100%)	6 (0%)	84	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	VAL
1	B	536	VAL
1	C	275	ARG
1	C	381	LEU
1	C	536	VAL
1	D	536	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	530	ASN
1	B	218	GLN
1	B	232	ASN
1	B	419	GLN
1	B	530	ASN
1	C	530	ASN
1	D	218	GLN
1	D	506	GLN
1	D	530	ASN
1	D	538	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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
4	SOG	A	604	-	20,20,20	1.94	2 (10%)	24,25,25	1.75	5 (20%)
4	SOG	D	605	-	20,20,20	1.62	3 (15%)	24,25,25	1.30	3 (12%)
3	GOL	D	602	-	5,5,5	0.84	0	5,5,5	1.04	0
3	GOL	B	603	-	5,5,5	1.11	0	5,5,5	0.69	0
2	HEM	A	601	5,1	50,50,50	1.61	9 (18%)	66,82,82	1.49	12 (18%)
3	GOL	C	604	-	5,5,5	1.13	0	5,5,5	0.81	0
3	GOL	C	603	-	5,5,5	0.65	0	5,5,5	1.35	1 (20%)
3	GOL	D	603	-	5,5,5	0.98	0	5,5,5	1.00	0
3	GOL	C	602	-	5,5,5	1.00	0	5,5,5	0.98	0
3	GOL	D	604	-	5,5,5	1.16	0	5,5,5	0.86	0
4	SOG	B	604	-	20,20,20	1.97	3 (15%)	24,25,25	1.55	3 (12%)
2	HEM	B	601	1	50,50,50	1.51	7 (14%)	66,82,82	1.26	7 (10%)
4	SOG	C	605	-	20,20,20	1.66	2 (10%)	24,25,25	1.58	3 (12%)
2	HEM	D	601	5,1	50,50,50	1.40	8 (16%)	66,82,82	1.13	7 (10%)
3	GOL	A	603	-	5,5,5	1.34	1 (20%)	5,5,5	0.97	0
3	GOL	B	602	-	5,5,5	0.94	0	5,5,5	0.98	0
3	GOL	A	602	-	5,5,5	1.01	0	5,5,5	1.15	0
2	HEM	C	601	5,1	50,50,50	1.43	7 (14%)	66,82,82	1.37	9 (13%)

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
4	SOG	A	604	-	-	7/11/31/31	0/1/1/1
4	SOG	D	605	-	-	6/11/31/31	0/1/1/1
3	GOL	D	602	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	603	-	-	4/4/4/4	-
2	HEM	A	601	5,1	-	2/14/54/54	-
3	GOL	C	604	-	-	4/4/4/4	-
3	GOL	C	603	-	-	2/4/4/4	-
3	GOL	D	603	-	-	0/4/4/4	-
3	GOL	C	602	-	-	1/4/4/4	-
3	GOL	D	604	-	-	0/4/4/4	-
4	SOG	B	604	-	-	9/11/31/31	0/1/1/1
2	HEM	B	601	1	-	2/14/54/54	-
4	SOG	C	605	-	-	5/11/31/31	0/1/1/1
2	HEM	D	601	5,1	-	0/14/54/54	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
2	HEM	C	601	5,1	-	2/14/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	SOG	O5-C1	6.68	1.52	1.42
4	A	604	SOG	O5-C1	6.55	1.52	1.42
4	C	605	SOG	O5-C1	5.38	1.50	1.42
4	D	605	SOG	O5-C1	4.96	1.50	1.42
2	A	601	HEM	FE-NB	4.89	2.10	1.94
2	B	601	HEM	FE-NA	4.87	2.11	1.95
2	B	601	HEM	FE-NB	4.79	2.09	1.94
2	C	601	HEM	FE-NB	4.41	2.08	1.94
2	A	601	HEM	FE-NC	4.25	2.09	1.95
4	B	604	SOG	C1'-S1	4.15	1.86	1.81
2	D	601	HEM	FE-NA	3.98	2.08	1.95
4	A	604	SOG	C1'-S1	3.70	1.86	1.81
2	A	601	HEM	FE-NA	3.46	2.06	1.95
2	D	601	HEM	FE-NB	3.25	2.04	1.94
2	C	601	HEM	CAC-C3C	3.15	1.56	1.47
4	C	605	SOG	C1'-S1	3.14	1.85	1.81
2	B	601	HEM	CAC-C3C	3.04	1.55	1.47
2	D	601	HEM	CAB-C3B	3.02	1.55	1.47
4	D	605	SOG	C1'-S1	2.92	1.85	1.81
2	A	601	HEM	CAB-C3B	2.90	1.55	1.47
2	A	601	HEM	FE-ND	2.89	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	FE-ND	2.89	2.03	1.94
2	A	601	HEM	CAC-C3C	2.84	1.55	1.47
2	C	601	HEM	FE-NC	2.82	2.04	1.95
2	B	601	HEM	CAB-C3B	2.77	1.55	1.47
2	D	601	HEM	CAC-C3C	2.74	1.54	1.47
2	C	601	HEM	CAB-C3B	2.73	1.54	1.47
4	D	605	SOG	C1-S1	-2.47	1.76	1.80
2	D	601	HEM	CMC-C2C	2.43	1.55	1.50
2	C	601	HEM	FE-NA	2.41	2.03	1.95
2	A	601	HEM	CMA-C3A	2.24	1.55	1.50
2	B	601	HEM	C2A-C3A	-2.21	1.32	1.38
2	B	601	HEM	CMC-C2C	2.18	1.55	1.50
2	A	601	HEM	O1A-CGA	2.11	1.29	1.22
2	D	601	HEM	CAA-C2A	2.11	1.56	1.51
2	A	601	HEM	CMD-C2D	2.11	1.55	1.50
2	C	601	HEM	CMD-C2D	2.09	1.55	1.50
2	D	601	HEM	FE-NC	2.07	2.02	1.95
2	B	601	HEM	CMB-C2B	2.05	1.55	1.50
3	A	603	GOL	C1-C2	2.05	1.60	1.51
2	D	601	HEM	CMB-C2B	2.04	1.55	1.50
4	B	604	SOG	O5-C5	2.02	1.49	1.44

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	605	SOG	C1'-S1-C1	5.77	110.87	100.09
4	B	604	SOG	C1'-S1-C1	5.66	110.68	100.09
4	A	604	SOG	O5-C1-C2	5.40	117.11	110.31
2	A	601	HEM	C4D-ND-C1D	3.98	109.19	105.07
2	A	601	HEM	CAA-CBA-CGA	-3.97	105.05	113.60
2	B	601	HEM	C4D-ND-C1D	3.94	109.14	105.07
2	A	601	HEM	C4C-NC-C1C	3.69	108.96	105.35
2	A	601	HEM	C1B-NB-C4B	3.66	108.85	105.07
2	C	601	HEM	C1B-NB-C4B	3.18	108.35	105.07
4	D	605	SOG	O5-C1-C2	3.15	114.27	110.31
4	D	605	SOG	C1'-S1-C1	3.13	105.95	100.09
4	A	604	SOG	C1'-S1-C1	3.04	105.77	100.09
2	C	601	HEM	CAA-CBA-CGA	-2.97	107.22	113.60
2	B	601	HEM	C2D-C1D-ND	-2.85	106.47	109.88
4	A	604	SOG	C1-C2-C3	2.83	116.17	110.59
2	C	601	HEM	O1A-CGA-CBA	-2.82	114.03	123.08
2	C	601	HEM	C4C-NC-C1C	2.81	108.10	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	SOG	C3-C4-C5	-2.70	105.42	110.24
2	C	601	HEM	O2A-CGA-CBA	2.66	122.57	114.03
2	A	601	HEM	CHD-C1D-ND	2.60	127.24	124.42
2	A	601	HEM	C3B-C2B-C1B	2.60	108.41	106.49
4	C	605	SOG	C1-O5-C5	-2.58	107.83	112.58
2	C	601	HEM	CAA-C2A-C1A	-2.57	119.83	124.89
2	A	601	HEM	C3D-C4D-ND	-2.52	107.36	110.17
4	A	604	SOG	O5-C5-C6	2.52	112.70	106.44
2	B	601	HEM	CBA-CAA-C2A	-2.45	105.81	112.63
2	C	601	HEM	C4D-ND-C1D	2.44	107.59	105.07
2	B	601	HEM	CBD-CAD-C3D	-2.39	105.99	112.63
2	A	601	HEM	C4A-NA-C1A	2.38	107.68	105.35
2	B	601	HEM	C4C-NC-C1C	2.38	107.67	105.35
4	A	604	SOG	C3-C4-C5	-2.33	106.08	110.24
2	B	601	HEM	C1B-NB-C4B	2.33	107.48	105.07
3	C	603	GOL	C3-C2-C1	-2.32	102.70	111.70
2	B	601	HEM	CHA-C4D-ND	2.31	127.22	124.37
2	D	601	HEM	C4D-ND-C1D	2.26	107.41	105.07
2	D	601	HEM	O2D-CGD-CBD	2.26	121.28	114.03
2	D	601	HEM	CHD-C1D-ND	2.25	126.86	124.42
2	D	601	HEM	C1B-NB-C4B	2.24	107.39	105.07
4	C	605	SOG	C4-C3-C2	2.23	114.72	110.82
2	D	601	HEM	C4A-NA-C1A	2.22	107.52	105.35
2	A	601	HEM	C2D-C1D-ND	-2.20	107.24	109.88
2	D	601	HEM	C4C-NC-C1C	2.19	107.50	105.35
2	A	601	HEM	O2D-CGD-CBD	2.13	120.86	114.03
2	A	601	HEM	C2B-C1B-NB	-2.09	107.36	109.84
2	C	601	HEM	CHA-C1A-NA	2.07	127.66	123.85
4	D	605	SOG	O5-C1-S1	-2.05	104.91	109.82
2	C	601	HEM	CHB-C1B-NB	2.05	126.90	124.37
2	A	601	HEM	C2A-C1A-NA	-2.03	107.88	110.15
4	B	604	SOG	O5-C5-C6	2.01	111.44	106.44
2	D	601	HEM	C3B-C2B-C1B	2.00	107.97	106.49

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	C	604	GOL	O1-C1-C2-C3
3	D	602	GOL	O1-C1-C2-C3
4	A	604	SOG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
4	B	604	SOG	O5-C1-S1-C1'
4	B	604	SOG	C2'-C1'-S1-C1
4	C	605	SOG	O5-C1-S1-C1'
4	D	605	SOG	O5-C1-S1-C1'
4	D	605	SOG	O5-C5-C6-O6
4	D	605	SOG	C4-C5-C6-O6
4	A	604	SOG	O5-C5-C6-O6
4	B	604	SOG	O5-C5-C6-O6
4	A	604	SOG	C4-C5-C6-O6
3	B	603	GOL	O1-C1-C2-O2
4	D	605	SOG	C2'-C3'-C4'-C5'
4	B	604	SOG	C3'-C4'-C5'-C6'
4	A	604	SOG	S1-C1'-C2'-C3'
3	B	603	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	C	603	GOL	C1-C2-C3-O3
3	C	604	GOL	C1-C2-C3-O3
4	B	604	SOG	C1'-C2'-C3'-C4'
4	C	605	SOG	C2'-C3'-C4'-C5'
3	C	604	GOL	O2-C2-C3-O3
3	D	602	GOL	O1-C1-C2-O2
4	C	605	SOG	C4'-C5'-C6'-C7'
4	B	604	SOG	C4'-C5'-C6'-C7'
4	B	604	SOG	C2'-C3'-C4'-C5'
4	B	604	SOG	S1-C1'-C2'-C3'
3	C	604	GOL	O1-C1-C2-O2
4	D	605	SOG	C3'-C4'-C5'-C6'
3	A	602	GOL	O1-C1-C2-O2
4	D	605	SOG	C5'-C6'-C7'-C8'
4	C	605	SOG	C3'-C4'-C5'-C6'
4	A	604	SOG	C2'-C1'-S1-C1
3	C	602	GOL	O1-C1-C2-O2
4	A	604	SOG	C2-C1-S1-C1'
4	A	604	SOG	C5'-C6'-C7'-C8'
3	B	603	GOL	O2-C2-C3-O3
3	C	603	GOL	O2-C2-C3-O3
4	B	604	SOG	C4-C5-C6-O6
3	D	602	GOL	C1-C2-C3-O3
2	C	601	HEM	CAD-CBD-CGD-O1D
2	C	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O1D

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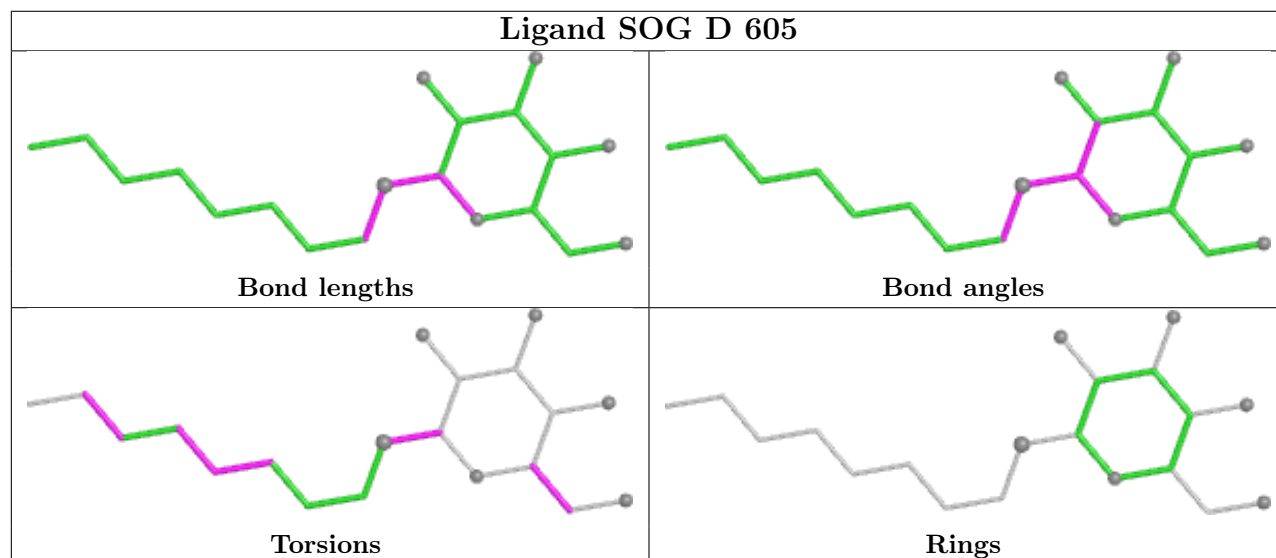
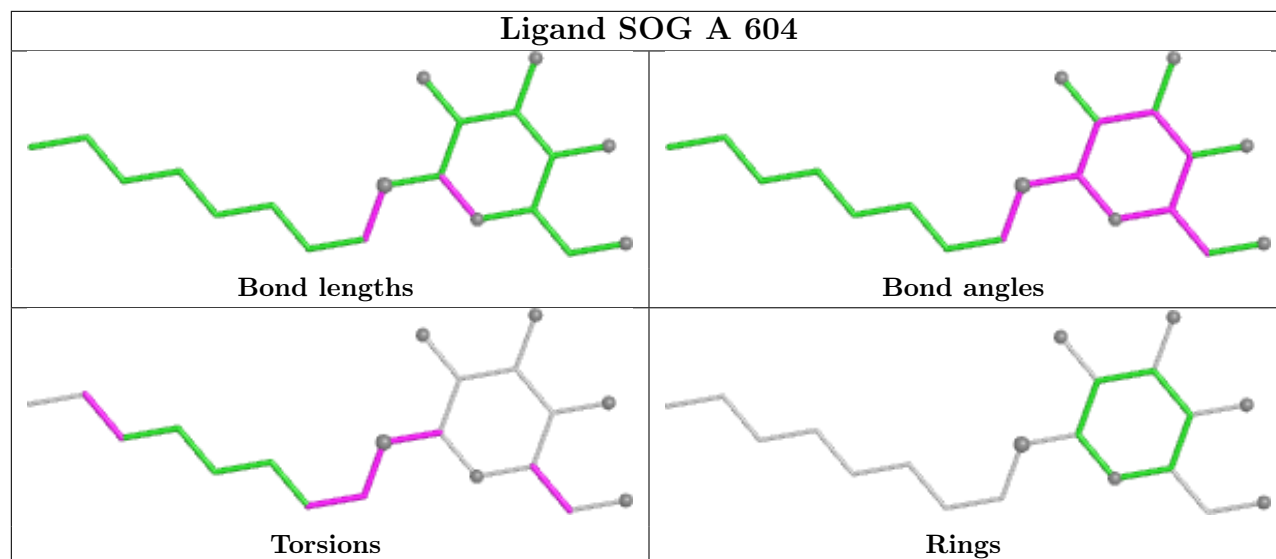
Mol	Chain	Res	Type	Atoms
2	A	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O2D
4	C	605	SOG	S1-C1'-C2'-C3'

There are no ring outliers.

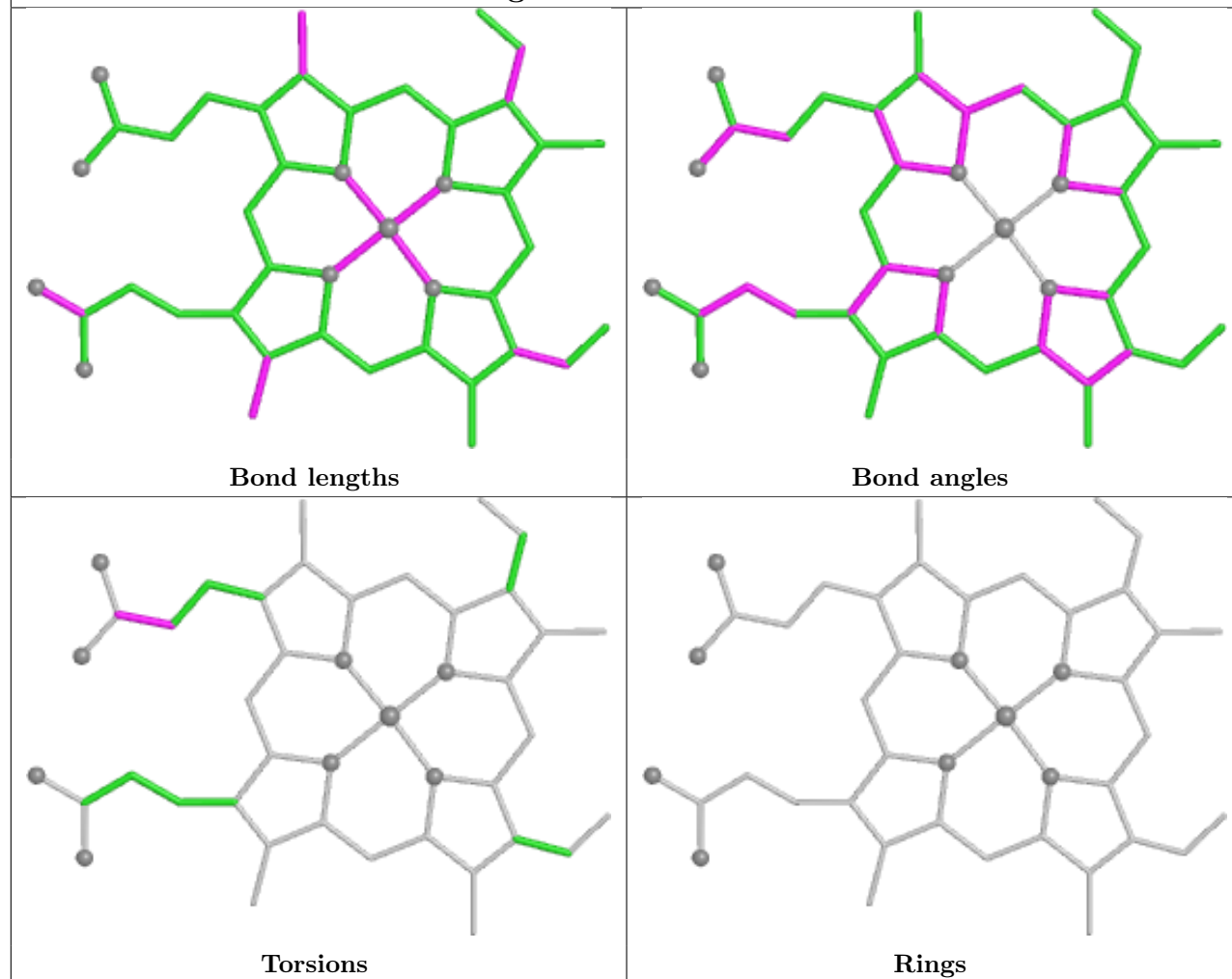
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	SOG	1	0
4	D	605	SOG	2	0
2	A	601	HEM	3	0
3	C	603	GOL	1	0
4	B	604	SOG	4	0
2	B	601	HEM	2	0
4	C	605	SOG	2	0
3	A	602	GOL	1	0

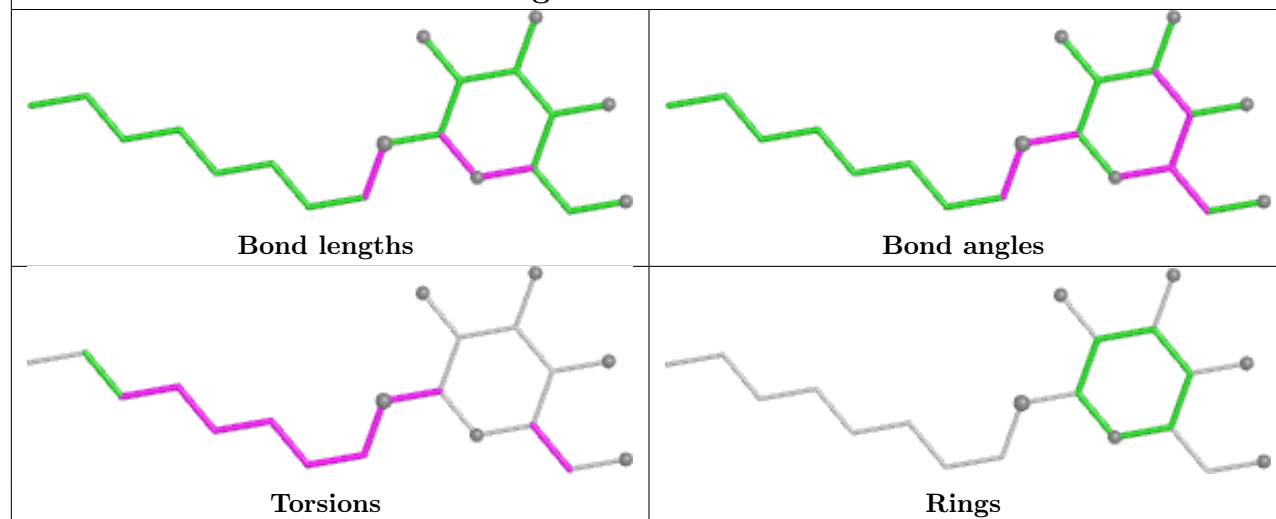
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

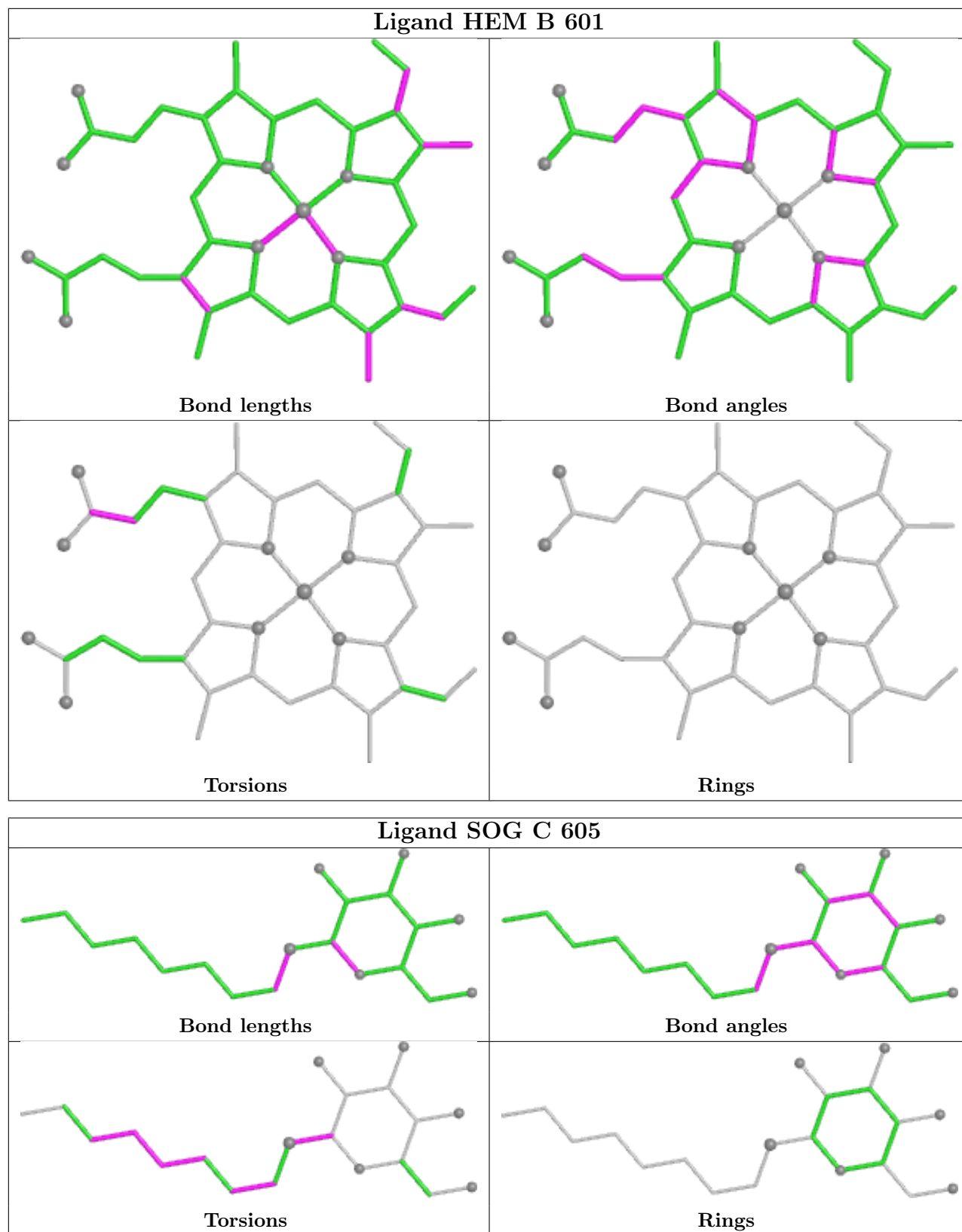


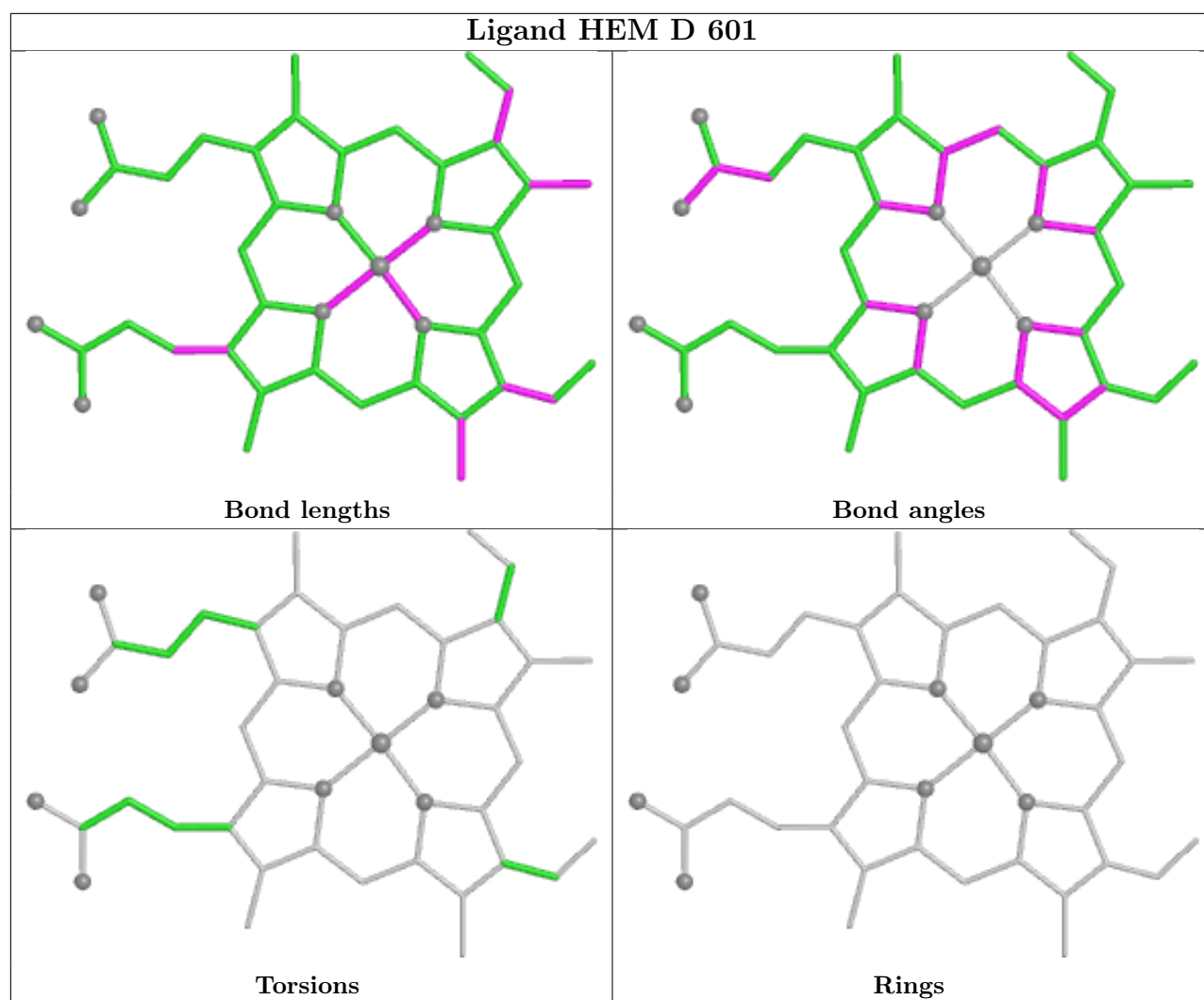
Ligand HEM A 601

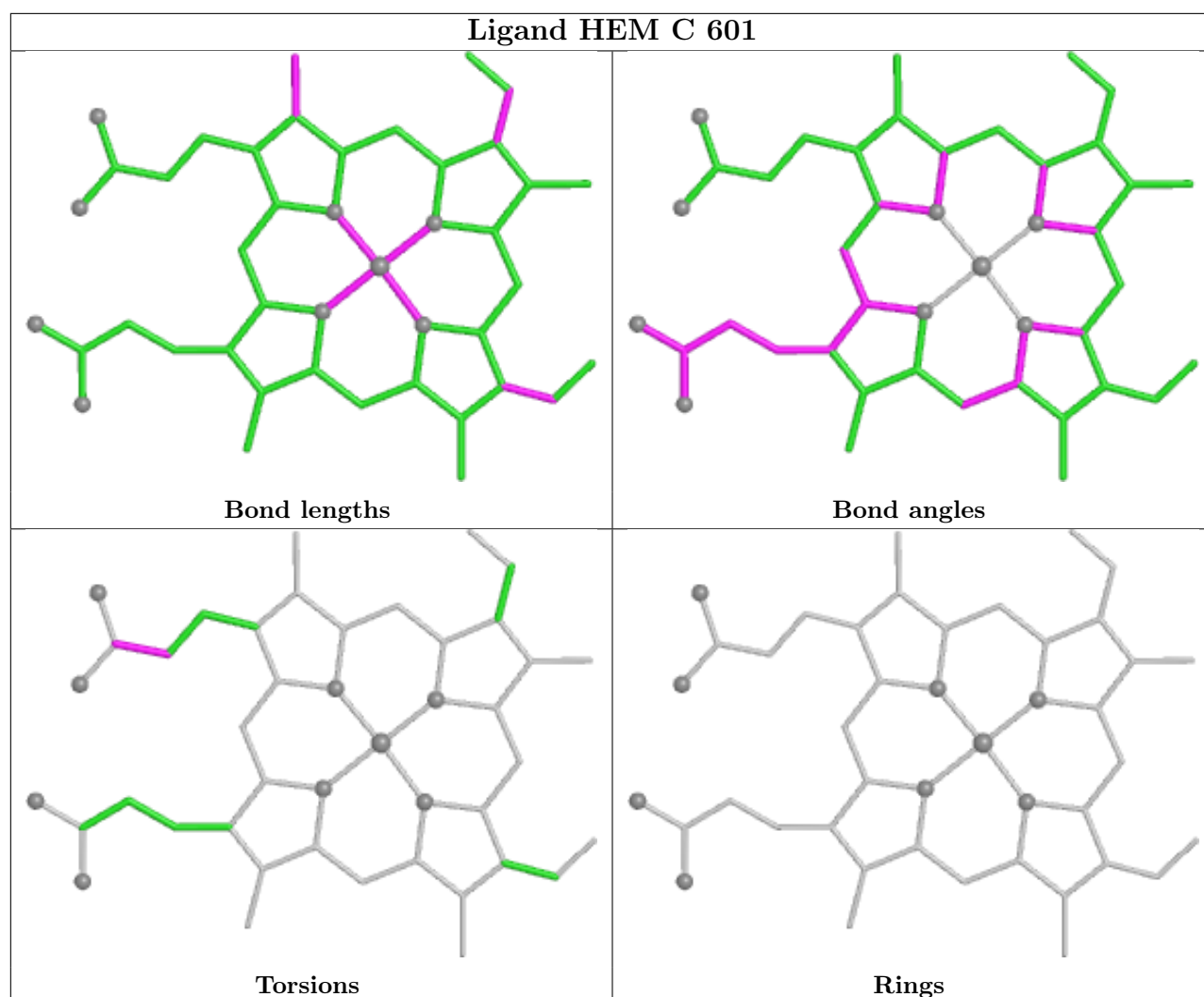


Ligand SOG B 604









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	466/471 (98%)	-0.58	0 100 100	11, 20, 33, 51	25 (5%)
1	B	465/471 (98%)	-0.11	8 (1%) 69 68	12, 29, 53, 90	13 (2%)
1	C	465/471 (98%)	-0.21	6 (1%) 75 74	15, 28, 49, 96	13 (2%)
1	D	466/471 (98%)	-0.03	7 (1%) 72 71	16, 32, 54, 97	8 (1%)
All	All	1862/1884 (98%)	-0.23	21 (1%) 78 77	11, 27, 49, 97	59 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	GLU	4.7
1	C	308	ILE	4.2
1	C	307	ARG	3.8
1	C	305	GLY	3.4
1	C	309	ASN	3.2
1	B	305	GLY	3.1
1	B	306	GLU	2.8
1	B	300	ILE	2.6
1	D	310	ASP	2.6
1	D	308	ILE	2.5
1	B	118	PRO	2.5
1	D	307	ARG	2.4
1	B	310	ASP	2.3
1	B	301	VAL	2.3
1	B	292	ASP	2.2
1	C	310	ASP	2.2
1	D	299	GLU	2.1
1	D	295	ALA	2.1
1	D	305	GLY	2.1
1	D	303	ARG	2.1
1	B	117	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

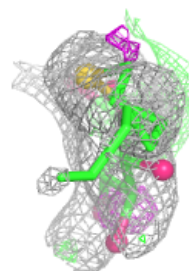
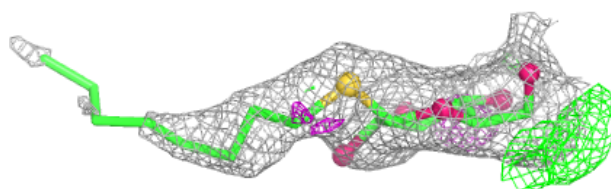
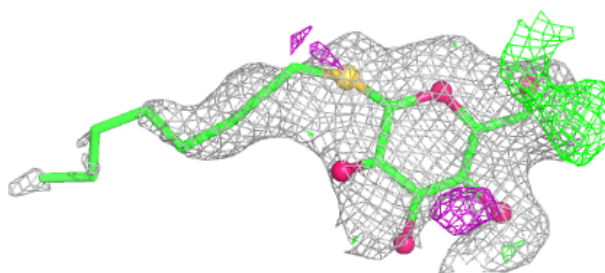
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	602	6/6	0.68	0.13	57,65,69,73	0
3	GOL	C	604	6/6	0.72	0.15	44,47,53,54	0
3	GOL	D	602	6/6	0.73	0.15	50,57,59,61	0
4	SOG	A	604	20/20	0.77	0.15	40,53,59,68	0
3	GOL	D	603	6/6	0.80	0.11	46,50,52,63	0
4	SOG	D	605	20/20	0.80	0.14	44,55,67,74	0
4	SOG	B	604	20/20	0.82	0.15	40,50,60,69	0
3	GOL	A	602	6/6	0.82	0.13	34,42,47,47	0
4	SOG	C	605	20/20	0.84	0.12	37,46,54,59	0
3	GOL	B	603	6/6	0.84	0.11	40,48,54,56	0
3	GOL	C	603	6/6	0.85	0.16	34,40,44,47	0
3	GOL	D	604	6/6	0.90	0.13	36,38,40,41	0
3	GOL	B	602	6/6	0.92	0.09	32,38,41,42	0
3	GOL	A	603	6/6	0.94	0.08	20,23,29,29	0
2	HEM	C	601	43/43	0.98	0.06	11,18,23,32	0
2	HEM	D	601	43/43	0.98	0.06	16,21,31,40	0
2	HEM	A	601	43/43	0.98	0.06	10,15,18,27	0
2	HEM	B	601	43/43	0.98	0.05	12,17,22,32	0

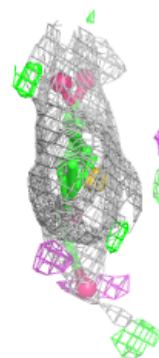
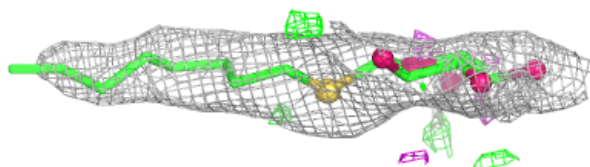
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SOG A 604:

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

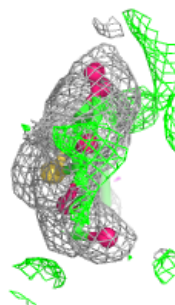
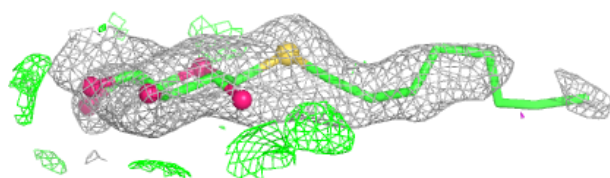
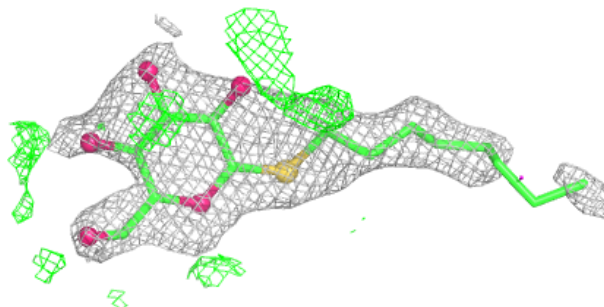
**Electron density around SOG D 605:**

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

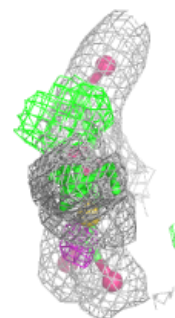
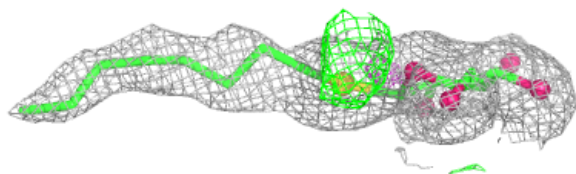
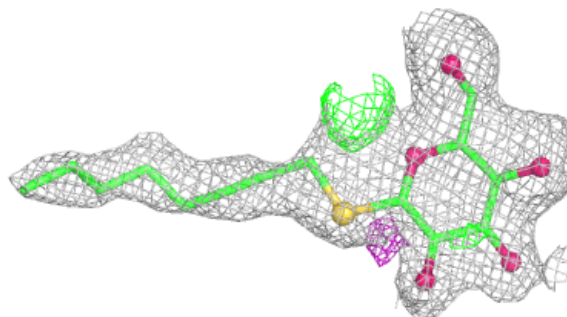


Electron density around SOG B 604:

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

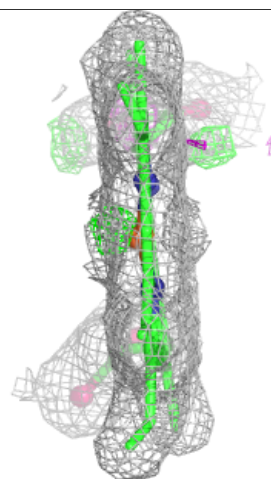
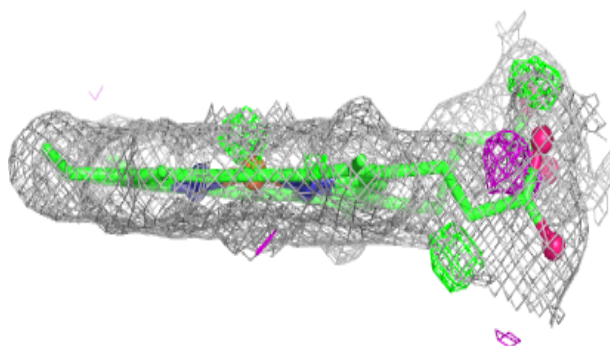
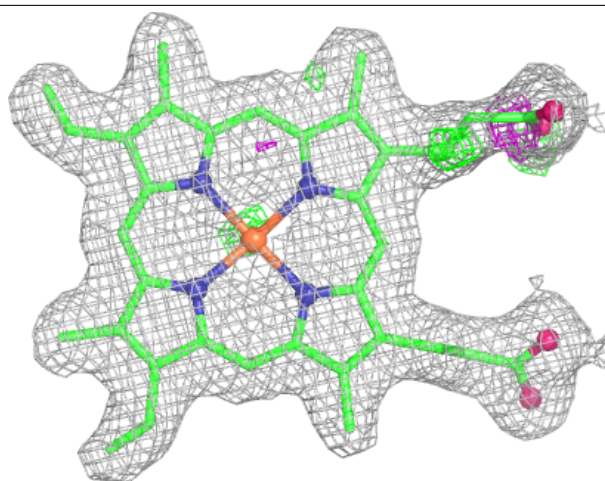
**Electron density around SOG C 605:**

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



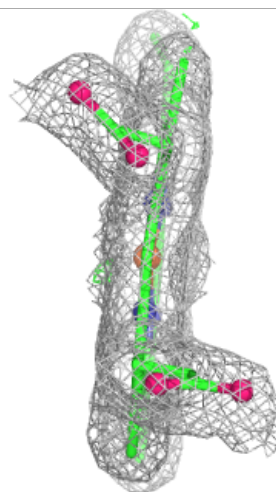
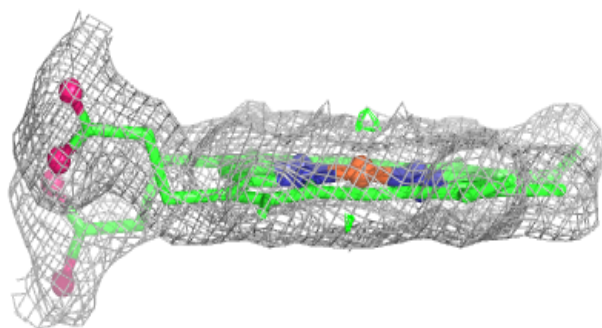
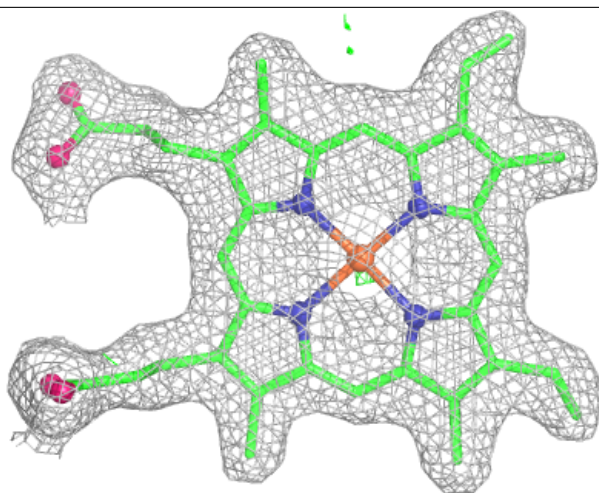
Electron density around HEM C 601:

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



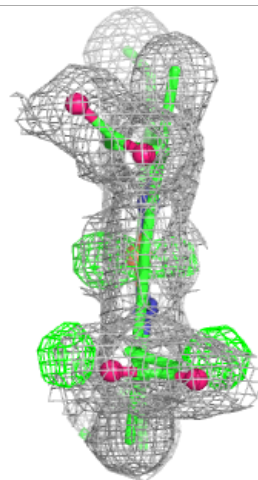
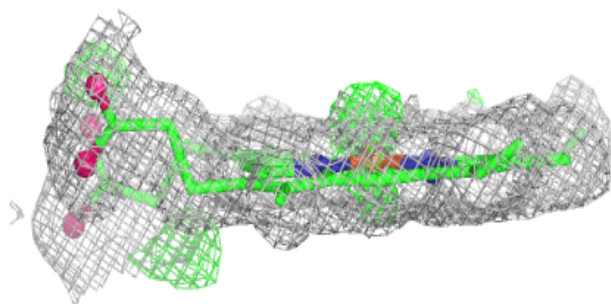
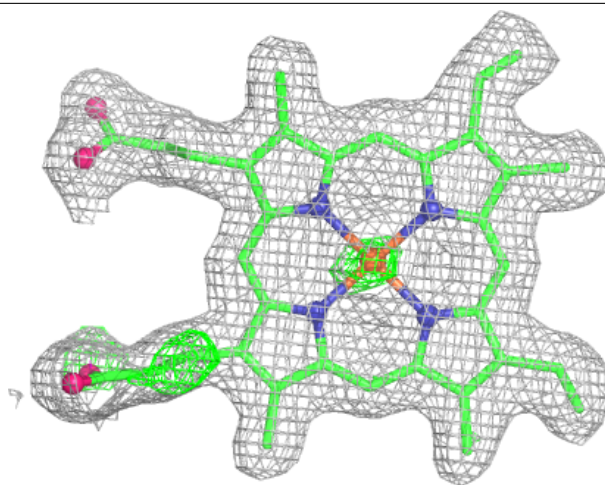
Electron density around HEM D 601:

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



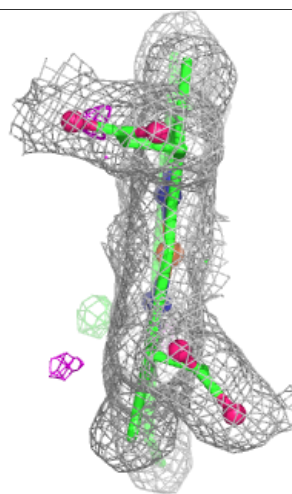
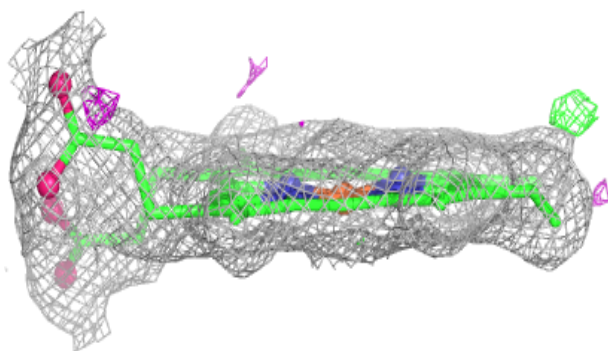
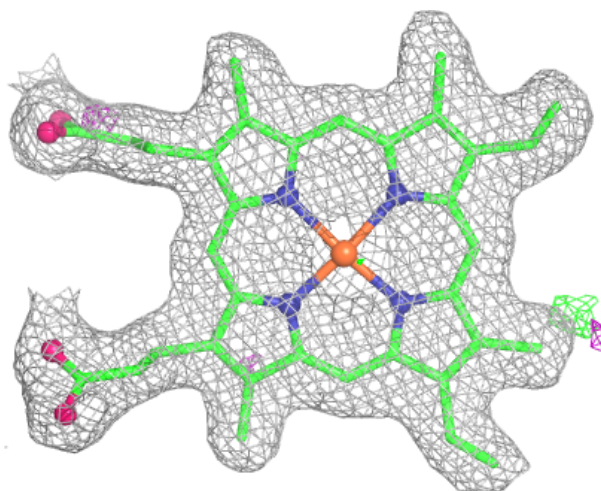
Electron density around HEM A 601:

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



Electron density around HEM B 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.