



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:15 AM UTC

PDB ID : 4XRY / pdb_00004xry
Title : Human Cytochrome P450 2D6 BACE1 Inhibitor 5 Complex
Authors : Johnson, E.F.; Fan, Y.
Deposited on : 2015-01-21
Resolution : 2.50 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

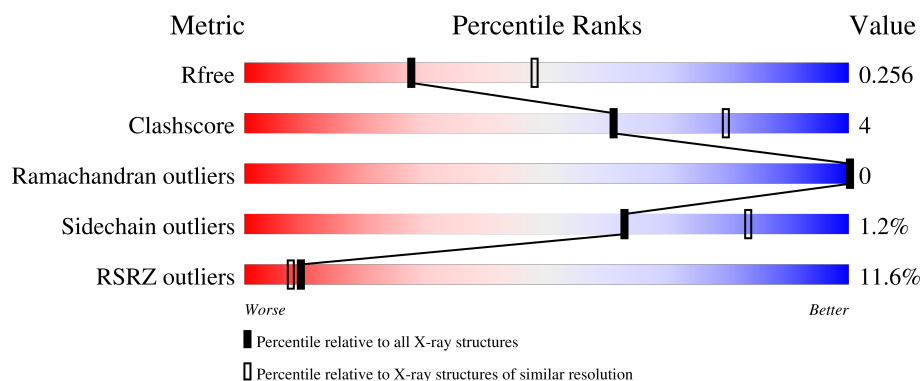
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	479	10% 88% 9% .
1	B	479	10% 84% 10% 5%
1	C	479	10% 83% 10% 7%
1	D	479	13% 82% 12% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14847 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3662	2349	649	650	14			
1	B	455	Total	C	N	O	S	0	0	0
			3602	2310	639	639	14			
1	C	446	Total	C	N	O	S	0	0	0
			3535	2267	625	629	14			
1	D	452	Total	C	N	O	S	0	0	0
			3577	2295	633	635	14			

There are 60 discrepancies between the modelled and reference sequences:

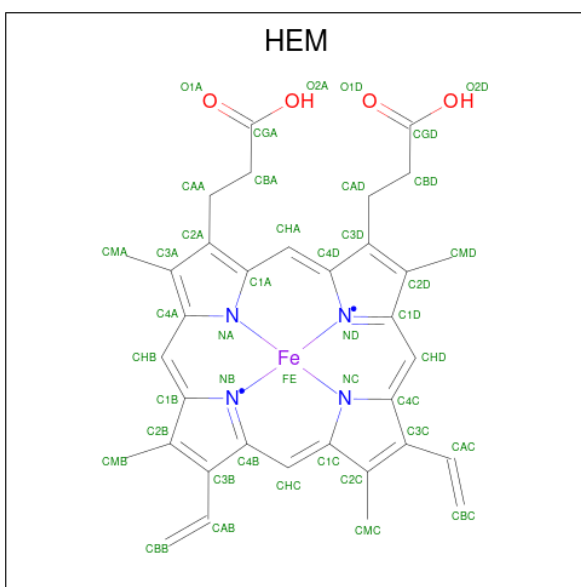
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	expression tag	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635

Continued on next page...

Continued from previous page...

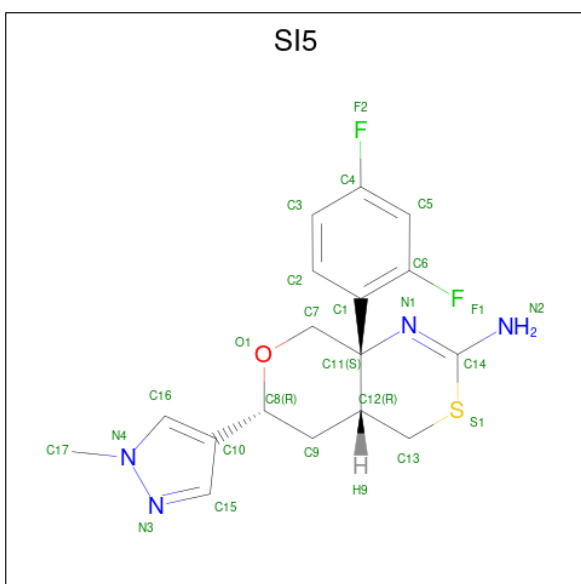
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	23	MET	-	expression tag	UNP P10635
C	24	ALA	-	expression tag	UNP P10635
C	25	LYS	-	expression tag	UNP P10635
C	26	LYS	-	expression tag	UNP P10635
C	27	THR	-	expression tag	UNP P10635
C	28	SER	-	expression tag	UNP P10635
C	29	SER	-	expression tag	UNP P10635
C	30	LYS	-	expression tag	UNP P10635
C	31	GLY	-	expression tag	UNP P10635
C	32	LYS	-	expression tag	UNP P10635
C	33	LEU	-	expression tag	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	23	MET	-	expression tag	UNP P10635
D	24	ALA	-	expression tag	UNP P10635
D	25	LYS	-	expression tag	UNP P10635
D	26	LYS	-	expression tag	UNP P10635
D	27	THR	-	expression tag	UNP P10635
D	28	SER	-	expression tag	UNP P10635
D	29	SER	-	expression tag	UNP P10635
D	30	LYS	-	expression tag	UNP P10635
D	31	GLY	-	expression tag	UNP P10635
D	32	LYS	-	expression tag	UNP P10635
D	33	LEU	-	expression tag	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635
D	501	HIS	-	expression tag	UNP P10635

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 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 (4aR,6R,8aS)-8a-(2,4-difluorophenyl)-6-(1-methyl-1H-pyrazol-4-yl)-4,4a,5,6,8,8a-hexahydropyrano[3,4-d][1,3]thiazin-2-amine (CCD ID: SI5) (formula: C₁₇H₁₈F₂N₄OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	
3	B	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	
3	C	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	
3	D	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Zn		
			4	4	0	0
4	B	3	Total	Zn		
			3	3	0	0
4	C	5	Total	Zn		
			5	5	0	0
4	D	5	Total	Zn		
			5	5	0	0

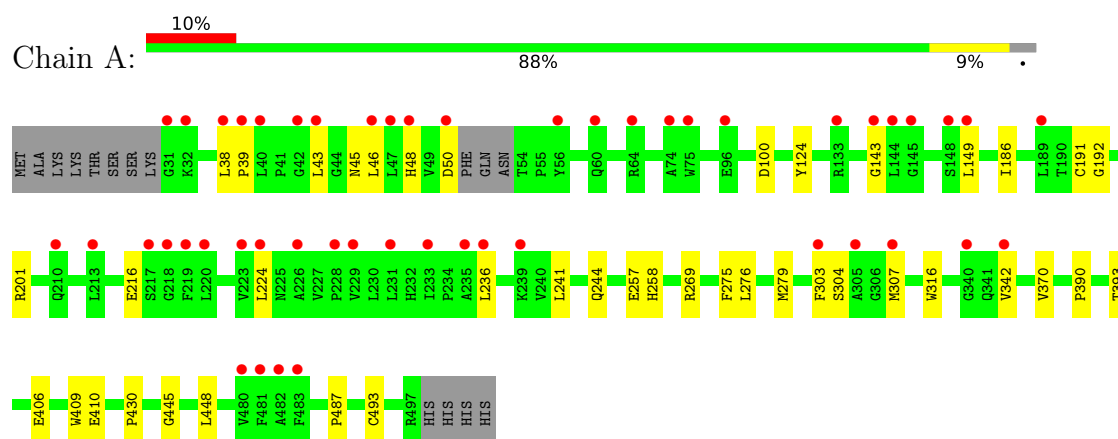
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O		
			54	54	0	0
5	B	43	Total	O		
			43	43	0	0
5	C	47	Total	O		
			47	47	0	0
5	D	38	Total	O		
			38	38	0	0

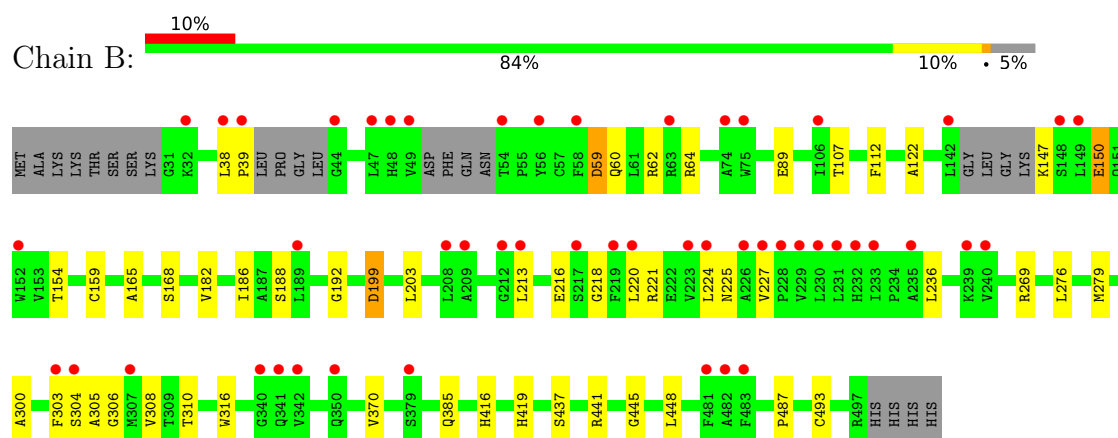
3 Residue-property plots [i](#)

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

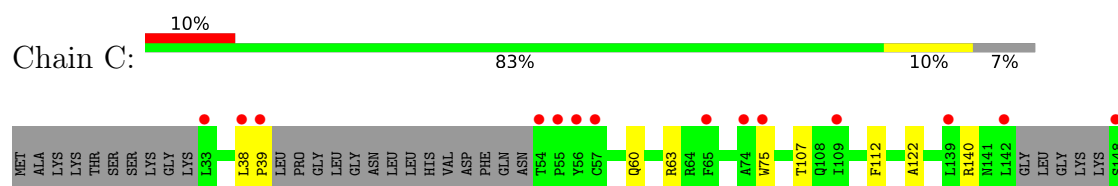
• Molecule 1: Cytochrome P450 2D6

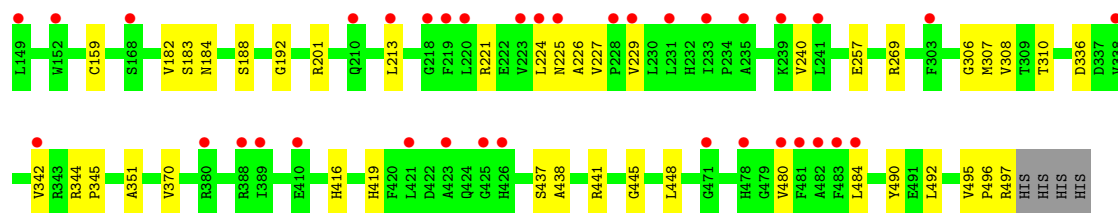


• Molecule 1: Cytochrome P450 2D6

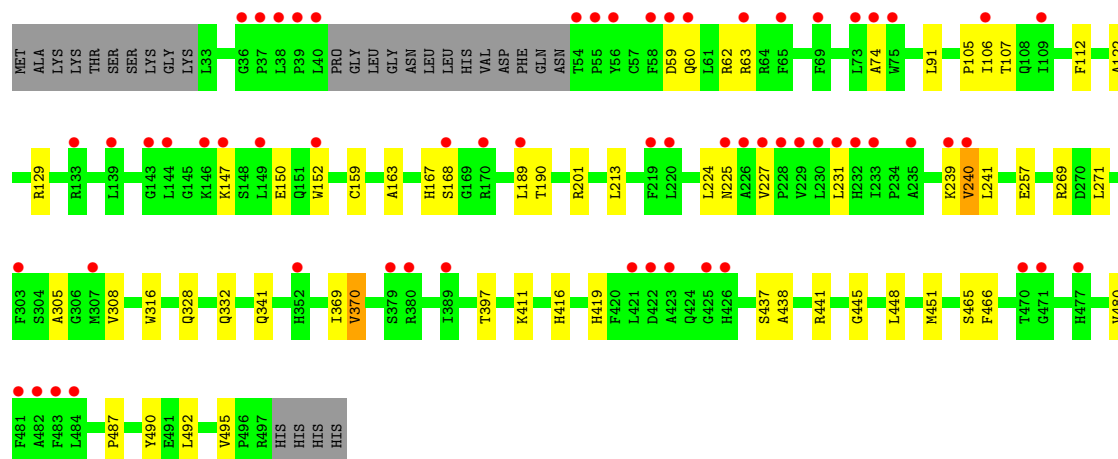
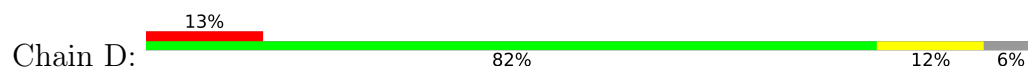


• Molecule 1: Cytochrome P450 2D6





● Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.06Å 192.34Å 247.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.50 39.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.16-2.50) 99.4 (39.16-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.208 , 0.251 0.218 , 0.256	Depositor DCC
R_{free} test set	4768 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14847	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 21.69 % 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 6.6474e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SI5, HEM, ZN

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	0.30	0/3760	0.74	0/5113
1	B	0.29	0/3697	0.73	2/5025 (0.0%)
1	C	0.29	0/3630	0.73	0/4938
1	D	0.29	0/3673	0.74	1/4995 (0.0%)
All	All	0.29	0/14760	0.73	3/20071 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ASP	CA-C-N	5.12	124.56	119.24
1	B	199	ASP	C-N-CA	5.12	124.56	119.24
1	D	74	ALA	CB-CA-C	-5.04	110.37	117.23

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	3662	0	3654	25	0
1	B	3602	0	3586	29	0
1	C	3535	0	3510	28	0
1	D	3577	0	3565	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	4	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0
2	D	43	0	30	4	0
3	A	25	0	18	1	0
3	B	25	0	18	1	0
3	C	25	0	18	0	0
3	D	25	0	18	2	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	54	0	0	1	0
5	B	43	0	0	2	0
5	C	47	0	0	3	0
5	D	38	0	0	3	0
All	All	14847	0	14507	122	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 4.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG21	1:A:303:PHE:HA	1.67	0.75
1:D:122:ALA:O	1:D:441:ARG:NH2	2.18	0.74
1:B:159:CYS:SG	5:B:713:HOH:O	2.44	0.74
1:C:122:ALA:O	1:C:441:ARG:NH2	2.18	0.74
1:B:493:CYS:SG	5:B:710:HOH:O	2.49	0.71
1:C:159:CYS:SG	5:C:715:HOH:O	2.51	0.69
1:B:186:ILE:HG21	1:B:303:PHE:HA	1.75	0.68
1:C:221:ARG:O	1:C:225:ASN:ND2	2.25	0.68
1:B:60:GLN:OE1	1:B:64:ARG:NH2	2.29	0.66
1:D:240:VAL:HG22	1:D:241:LEU:HG	1.79	0.65
1:D:416:HIS:ND1	5:D:715:HOH:O	2.29	0.65
1:C:60:GLN:OE1	1:C:63:ARG:NH1	2.31	0.63
1:B:38:LEU:HD12	1:B:39:PRO:HD2	1.83	0.61
1:C:140:ARG:NH1	5:C:744:HOH:O	2.29	0.60
1:C:224:LEU:HD12	1:C:240:VAL:HG11	1.82	0.60
1:D:147:LYS:HG2	1:D:150:GLU:HB2	1.84	0.59
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:SER:HA	1:A:307:MET:HE2	1.86	0.57
1:A:192:GLY:O	1:A:269:ARG:NH2	2.33	0.57
1:D:159:CYS:SG	5:D:712:HOH:O	2.58	0.56
1:D:437:SER:HB3	2:D:601:HEM:HBA1	1.86	0.56
1:D:437:SER:OG	1:D:438:ALA:N	2.35	0.56
1:A:493:CYS:SG	5:A:730:HOH:O	2.57	0.55
1:B:122:ALA:O	1:B:441:ARG:NH2	2.18	0.54
1:C:437:SER:HB3	2:C:601:HEM:HBA1	1.89	0.54
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.90	0.53
1:C:213:LEU:HD11	1:C:484:LEU:HD12	1.91	0.53
1:B:216:GLU:HA	1:B:221:ARG:HD3	1.90	0.53
1:C:227:VAL:HG12	1:C:229:VAL:HG22	1.91	0.53
1:C:437:SER:OG	1:C:438:ALA:N	2.34	0.52
1:D:213:LEU:HD12	3:D:602:SI5:H4	1.91	0.52
1:A:241:LEU:HB3	1:A:244:GLN:HB2	1.92	0.52
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.91	0.52
1:B:300:ALA:O	1:B:304:SER:OG	2.27	0.52
1:A:43:LEU:HD23	1:A:46:LEU:HD22	1.91	0.51
1:D:106:ILE:HD12	1:D:241:LEU:HD11	1.92	0.51
1:C:184:ASN:O	1:C:188:SER:OG	2.24	0.51
1:B:192:GLY:O	1:B:269:ARG:NH2	2.41	0.51
1:C:183:SER:OG	1:C:307:MET:HG3	2.10	0.51
2:D:601:HEM:HMB2	2:D:601:HEM:HBB2	1.91	0.51
1:C:445:GLY:HA3	2:C:601:HEM:C3C	2.47	0.50
1:C:336:ASP:OD2	1:C:497:ARG:NH2	2.43	0.50
1:A:191:CYS:HA	1:A:258:HIS:CE1	2.47	0.49
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.94	0.49
1:B:437:SER:HB3	2:B:601:HEM:HBA1	1.94	0.49
1:D:59:ASP:O	1:D:63:ARG:HG2	2.13	0.49
1:B:448:LEU:HD23	2:B:601:HEM:HBC2	1.94	0.48
1:D:129:ARG:NH1	5:D:732:HOH:O	2.45	0.48
1:D:201:ARG:NH1	1:D:257:GLU:OE1	2.32	0.48
1:D:448:LEU:HD23	2:D:601:HEM:HBC2	1.96	0.48
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.95	0.47
1:D:316:TRP:CD2	1:D:487:PRO:HG3	2.50	0.47
1:A:224:LEU:HD21	1:A:236:LEU:HD13	1.96	0.47
1:B:147:LYS:HE3	1:B:150:GLU:HB2	1.96	0.47
1:D:490:TYR:HE1	1:D:492:LEU:HD23	1.80	0.47
1:A:50:ASP:OD2	1:D:60:GLN:NE2	2.49	0.46
1:B:182:VAL:HG11	1:B:310:THR:HB	1.96	0.46
1:B:107:THR:HB	1:B:112:PHE:CG	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LEU:HD22	1:A:244:GLN:HG3	1.97	0.46
1:A:38:LEU:HA	1:A:39:PRO:HD3	1.77	0.46
1:C:192:GLY:O	1:C:269:ARG:NH2	2.49	0.45
1:C:201:ARG:NH1	1:C:257:GLU:OE1	2.39	0.45
1:D:213:LEU:HD13	1:D:308:VAL:HG21	1.98	0.45
1:B:221:ARG:O	1:B:225:ASN:HB2	2.16	0.45
1:A:390:PRO:O	1:A:393:THR:OG1	2.33	0.45
1:B:89:GLU:OE2	1:B:385:GLN:NE2	2.39	0.45
1:C:182:VAL:HG11	1:C:310:THR:HB	1.99	0.45
1:A:276:LEU:HA	1:A:279:MET:HE3	1.98	0.45
1:A:216:GLU:OE2	3:A:602:SI5:N2	2.42	0.44
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.98	0.44
1:C:75:TRP:CZ2	1:C:226:ALA:HB2	2.52	0.44
1:C:306:GLY:HA2	2:C:601:HEM:C2C	2.53	0.44
1:C:490:TYR:HE1	1:C:492:LEU:HD23	1.83	0.44
1:D:328:GLN:OE1	1:D:466:PHE:N	2.43	0.44
2:C:601:HEM:HBC2	2:C:601:HEM:HMC2	2.00	0.44
1:D:316:TRP:CG	1:D:487:PRO:HG3	2.52	0.44
1:D:163:ALA:O	1:D:167:HIS:ND1	2.40	0.44
1:B:218:GLY:C	1:B:220:LEU:H	2.26	0.44
1:A:100:ASP:HA	1:A:124:TYR:HB2	1.99	0.44
1:B:305:ALA:HB2	3:B:602:SI5:H8	2.00	0.44
1:D:224:LEU:HB3	1:D:231:LEU:HD21	2.00	0.43
1:C:107:THR:HB	1:C:112:PHE:CG	2.53	0.43
1:D:416:HIS:HB3	1:D:419:HIS:CE1	2.53	0.43
1:A:410:GLU:O	1:D:411:LYS:NZ	2.46	0.43
1:A:143:GLY:HA2	1:A:149:LEU:HD13	1.99	0.43
1:B:213:LEU:HD22	1:B:308:VAL:HG21	1.99	0.43
1:A:45:ASN:HA	1:A:48:HIS:HD2	1.84	0.43
1:C:495:VAL:HA	1:C:496:PRO:HD3	1.88	0.43
1:B:224:LEU:HD11	1:B:236:LEU:HD23	1.99	0.43
1:D:190:THR:HA	1:D:271:LEU:HB3	2.01	0.43
1:D:465:SER:HB3	1:D:495:VAL:HG23	2.01	0.43
1:C:213:LEU:HD13	1:C:308:VAL:HG21	2.00	0.42
1:A:406:GLU:O	1:D:411:LYS:HE3	2.19	0.42
1:B:445:GLY:HA3	2:B:601:HEM:C3C	2.54	0.42
1:C:416:HIS:HB3	1:C:419:HIS:CE1	2.53	0.42
1:B:165:ALA:O	1:B:168:SER:OG	2.27	0.42
1:B:416:HIS:HB3	1:B:419:HIS:CE1	2.54	0.42
1:B:199:ASP:O	1:B:203:LEU:HG	2.20	0.42
1:C:38:LEU:HD12	1:C:39:PRO:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:TRP:CD2	1:B:487:PRO:HG3	2.54	0.42
1:B:59:ASP:HA	1:B:62:ARG:HG2	2.02	0.42
1:C:344:ARG:HA	1:C:345:PRO:HD3	1.92	0.41
1:D:332:GLN:HE22	1:D:465:SER:HA	1.86	0.41
1:B:276:LEU:HA	1:B:279:MET:HE3	2.02	0.41
1:A:409:TRP:CZ3	1:A:430:PRO:HG2	2.55	0.41
1:A:448:LEU:HD23	2:A:601:HEM:HBC2	2.02	0.41
1:A:275:PHE:CD2	1:A:279:MET:HE2	2.56	0.41
1:A:316:TRP:CG	1:A:487:PRO:HG3	2.56	0.41
1:B:150:GLU:O	1:B:154:THR:HG23	2.21	0.41
1:B:306:GLY:HA2	2:B:601:HEM:C2C	2.55	0.41
1:C:351:ALA:N	5:C:724:HOH:O	2.45	0.41
1:D:91:LEU:HD11	1:D:397:THR:HG21	2.02	0.41
1:D:445:GLY:HA3	2:D:601:HEM:C3C	2.56	0.41
1:D:451:MET:HE3	1:D:451:MET:HB2	1.95	0.41
1:A:445:GLY:HA3	2:A:601:HEM:C3C	2.55	0.40
1:D:107:THR:HB	1:D:112:PHE:CG	2.55	0.40
1:D:239:LYS:HE2	1:D:239:LYS:HB3	1.84	0.40
1:A:201:ARG:HH12	1:A:257:GLU:CD	2.26	0.40
1:C:448:LEU:HD23	2:C:601:HEM:HBC2	2.03	0.40
1:D:152:TRP:CZ3	1:D:189:LEU:HD23	2.56	0.40
1:D:305:ALA:HB2	3:D:602:SI5:H8	2.03	0.40
1:D:105:PRO:HD2	1:D:225:ASN:OD1	2.22	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	460/479 (96%)	446 (97%)	14 (3%)	0	100	100
1	B	447/479 (93%)	437 (98%)	10 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	440/479 (92%)	427 (97%)	13 (3%)	0	100	100
1	D	448/479 (94%)	435 (97%)	13 (3%)	0	100	100
All	All	1795/1916 (94%)	1745 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/409 (97%)	393 (100%)	2 (0%)	81	92
1	B	389/409 (95%)	384 (99%)	5 (1%)	61	82
1	C	382/409 (93%)	379 (99%)	3 (1%)	73	88
1	D	386/409 (94%)	378 (98%)	8 (2%)	47	74
All	All	1552/1636 (95%)	1534 (99%)	18 (1%)	63	83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	VAL
1	A	370	VAL
1	B	59	ASP
1	B	150	GLU
1	B	188	SER
1	B	227	VAL
1	B	370	VAL
1	C	342	VAL
1	C	370	VAL
1	C	480	VAL
1	D	62	ARG
1	D	168	SER
1	D	227	VAL
1	D	240	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	269	ARG
1	D	341	GLN
1	D	370	VAL
1	D	480	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	94	HIS
1	A	341	GLN
1	B	94	HIS
1	C	94	HIS
1	C	166	ASN
1	C	332	GLN
1	C	350	GLN
1	D	266	GLN
1	D	424	GLN
1	D	478	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 17 are monoatomic - leaving 8 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
2	HEM	C	601	1	50,50,50	1.35	6 (12%)	67,82,82	1.13	6 (8%)
2	HEM	B	601	5,1	50,50,50	1.43	6 (12%)	67,82,82	1.08	4 (5%)
3	SI5	C	602	-	25,28,28	0.86	2 (8%)	26,42,42	1.02	2 (7%)
3	SI5	A	602	-	25,28,28	0.92	2 (8%)	26,42,42	1.00	2 (7%)
2	HEM	D	601	5,1	50,50,50	1.37	6 (12%)	67,82,82	1.07	3 (4%)
3	SI5	B	602	-	25,28,28	0.85	1 (4%)	26,42,42	1.13	3 (11%)
2	HEM	A	601	1	50,50,50	1.38	6 (12%)	67,82,82	1.12	5 (7%)
3	SI5	D	602	-	25,28,28	0.83	1 (4%)	26,42,42	1.10	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	601	1	-	2/14/54/54	-
2	HEM	B	601	5,1	-	2/14/54/54	-
3	SI5	C	602	-	-	0/10/36/36	0/4/4/4
3	SI5	A	602	-	-	0/10/36/36	0/4/4/4
2	HEM	D	601	5,1	-	0/14/54/54	-
3	SI5	B	602	-	-	0/10/36/36	0/4/4/4
2	HEM	A	601	1	-	3/14/54/54	-
3	SI5	D	602	-	-	0/10/36/36	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	FE-NB	4.07	2.07	1.94
2	B	601	HEM	FE-NA	4.06	2.08	1.95
2	B	601	HEM	FE-ND	3.94	2.07	1.94
2	D	601	HEM	FE-NC	3.88	2.08	1.95
2	B	601	HEM	FE-NB	3.82	2.06	1.94
2	A	601	HEM	FE-ND	3.77	2.06	1.94
2	C	601	HEM	FE-NC	3.59	2.07	1.95
2	D	601	HEM	FE-ND	3.56	2.05	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NA	3.49	2.06	1.95
2	A	601	HEM	FE-NC	3.49	2.06	1.95
2	A	601	HEM	FE-NB	3.49	2.05	1.94
2	D	601	HEM	FE-NB	3.37	2.05	1.94
2	B	601	HEM	FE-NC	3.29	2.06	1.95
2	D	601	HEM	FE-NA	3.26	2.05	1.95
2	C	601	HEM	FE-NA	3.24	2.05	1.95
3	A	602	SI5	N4-N3	3.18	1.39	1.35
2	B	601	HEM	CAC-C3C	3.14	1.55	1.47
2	D	601	HEM	CAC-C3C	3.12	1.55	1.47
2	C	601	HEM	CAC-C3C	3.09	1.55	1.47
2	D	601	HEM	CAB-C3B	3.05	1.55	1.47
2	B	601	HEM	CAB-C3B	3.04	1.55	1.47
2	A	601	HEM	CAC-C3C	3.04	1.55	1.47
2	C	601	HEM	CAB-C3B	3.03	1.55	1.47
2	A	601	HEM	CAB-C3B	2.97	1.55	1.47
2	C	601	HEM	FE-ND	2.74	2.03	1.94
3	B	602	SI5	N4-N3	2.70	1.38	1.35
3	C	602	SI5	N4-N3	2.65	1.38	1.35
3	D	602	SI5	N4-N3	2.57	1.38	1.35
3	C	602	SI5	C14-N1	2.08	1.31	1.27
3	A	602	SI5	C14-N1	2.06	1.31	1.27

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	C1B-NB-C4B	2.64	108.33	105.21
3	B	602	SI5	C12-C11-N1	2.60	113.98	109.70
2	A	601	HEM	C1B-NB-C4B	2.56	108.23	105.21
3	A	602	SI5	C12-C11-N1	2.55	113.90	109.70
2	C	601	HEM	C4D-ND-C1D	2.55	108.22	105.21
3	B	602	SI5	O1-C8-C9	-2.55	107.86	111.16
3	D	602	SI5	C12-C11-N1	2.51	113.83	109.70
3	C	602	SI5	C12-C11-N1	2.44	113.71	109.70
2	D	601	HEM	C1B-NB-C4B	2.42	108.07	105.21
2	C	601	HEM	C1B-NB-C4B	2.40	108.05	105.21
2	D	601	HEM	C3B-C2B-C1B	2.39	108.21	106.41
2	C	601	HEM	C3D-C4D-ND	-2.38	107.57	110.17
2	A	601	HEM	C4D-ND-C1D	2.35	107.99	105.21
2	A	601	HEM	C2A-C1A-NA	-2.33	107.57	110.15
2	A	601	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	C	601	HEM	C3B-C2B-C1B	2.26	108.11	106.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	SI5	O1-C8-C9	-2.23	108.28	111.16
2	D	601	HEM	C4D-ND-C1D	2.22	107.84	105.21
2	A	601	HEM	CAA-CBA-CGA	-2.19	107.84	113.67
2	B	601	HEM	C4D-ND-C1D	2.13	107.73	105.21
3	A	602	SI5	O1-C8-C9	-2.12	108.41	111.16
2	C	601	HEM	C2A-C1A-NA	-2.10	107.82	110.15
2	B	601	HEM	C3B-C2B-C1B	2.07	107.97	106.41
3	C	602	SI5	O1-C8-C9	-2.06	108.49	111.16
2	B	601	HEM	CAA-CBA-CGA	-2.05	108.24	113.67
2	C	601	HEM	CAA-CBA-CGA	-2.03	108.27	113.67
3	B	602	SI5	C7-C11-C1	-2.03	107.29	111.39
3	D	602	SI5	C7-C11-C1	-2.01	107.33	111.39

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O2D

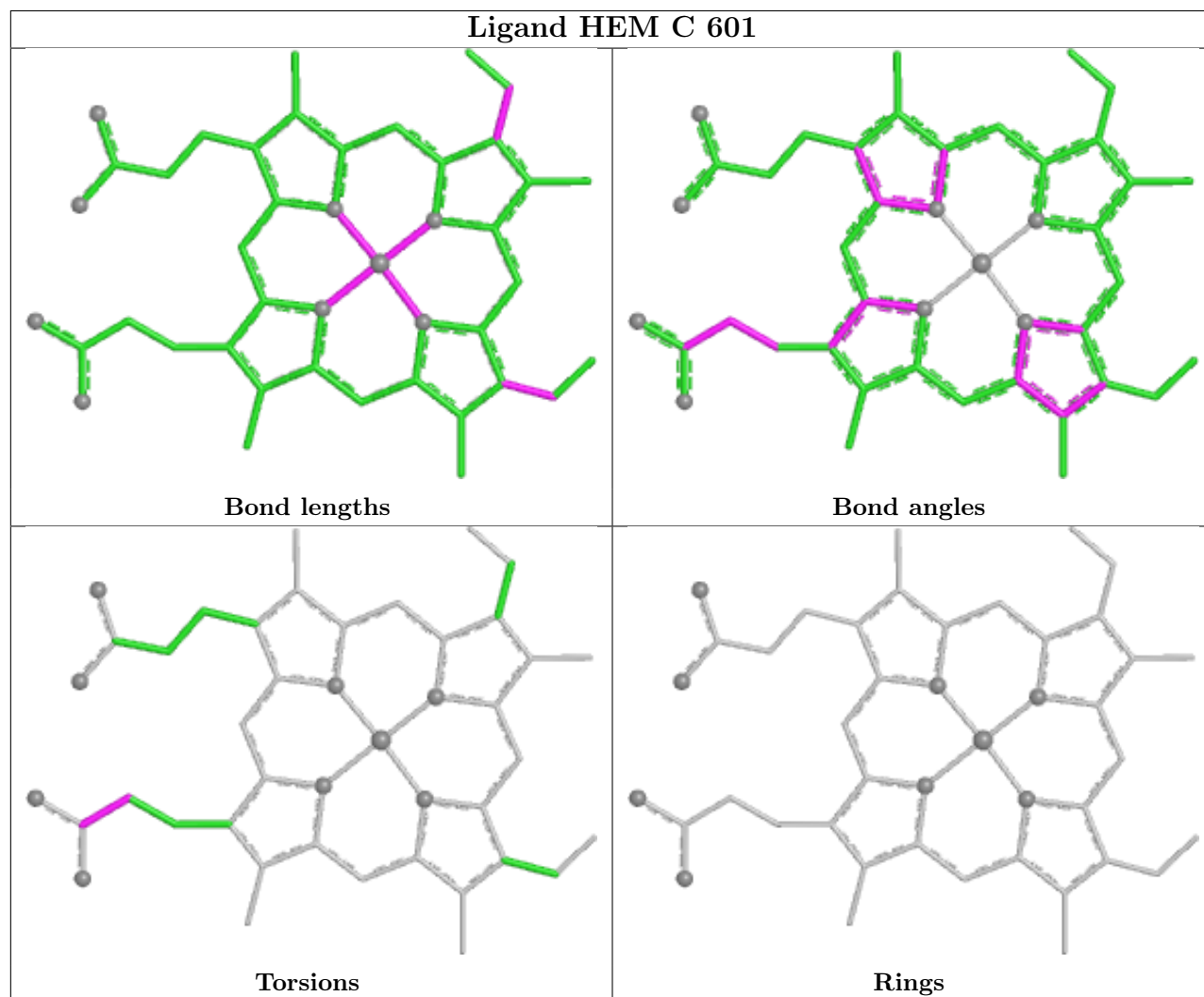
There are no ring outliers.

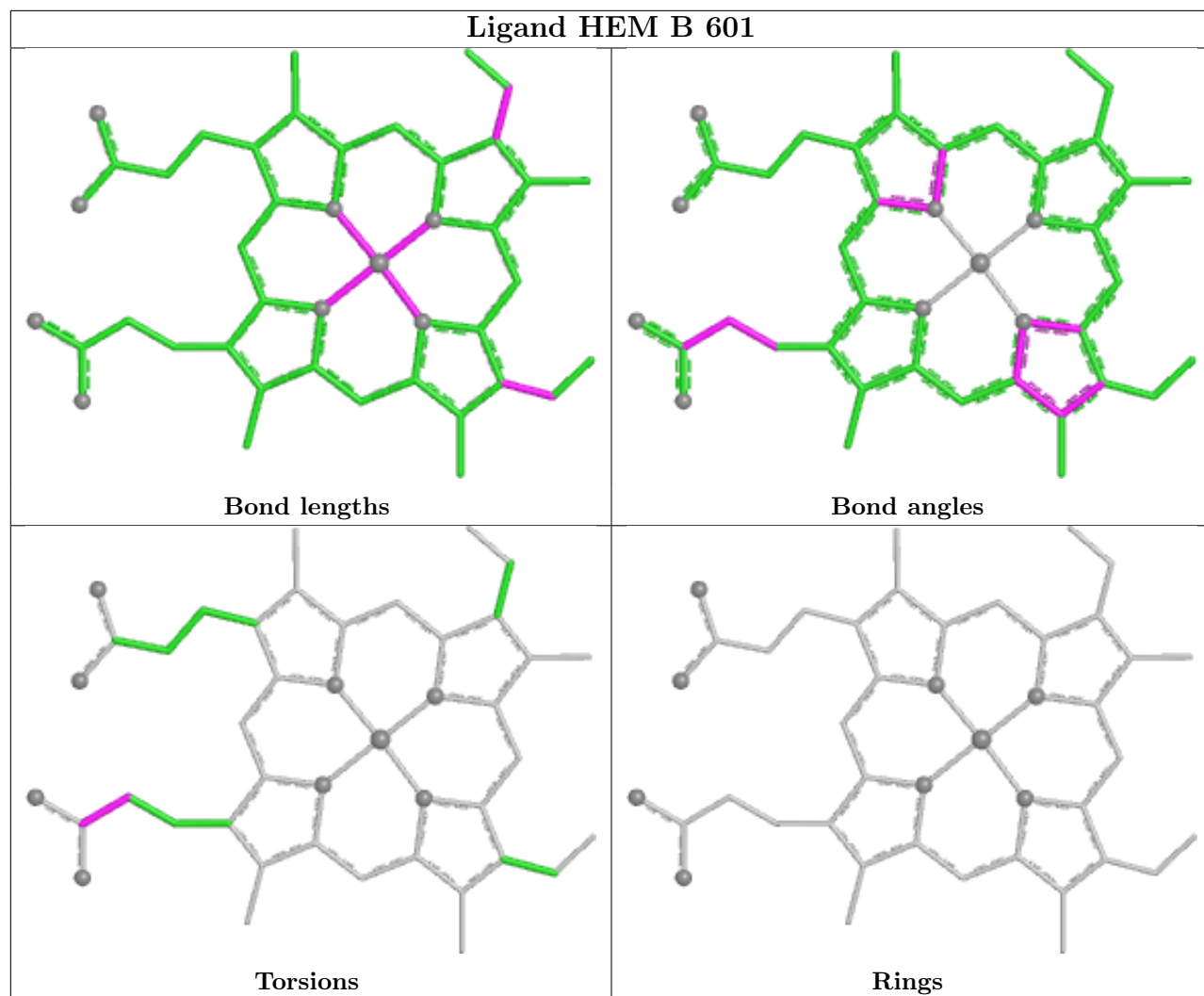
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	6	0
2	B	601	HEM	6	0
3	A	602	SI5	1	0
2	D	601	HEM	4	0
3	B	602	SI5	1	0
2	A	601	HEM	4	0
3	D	602	SI5	2	0

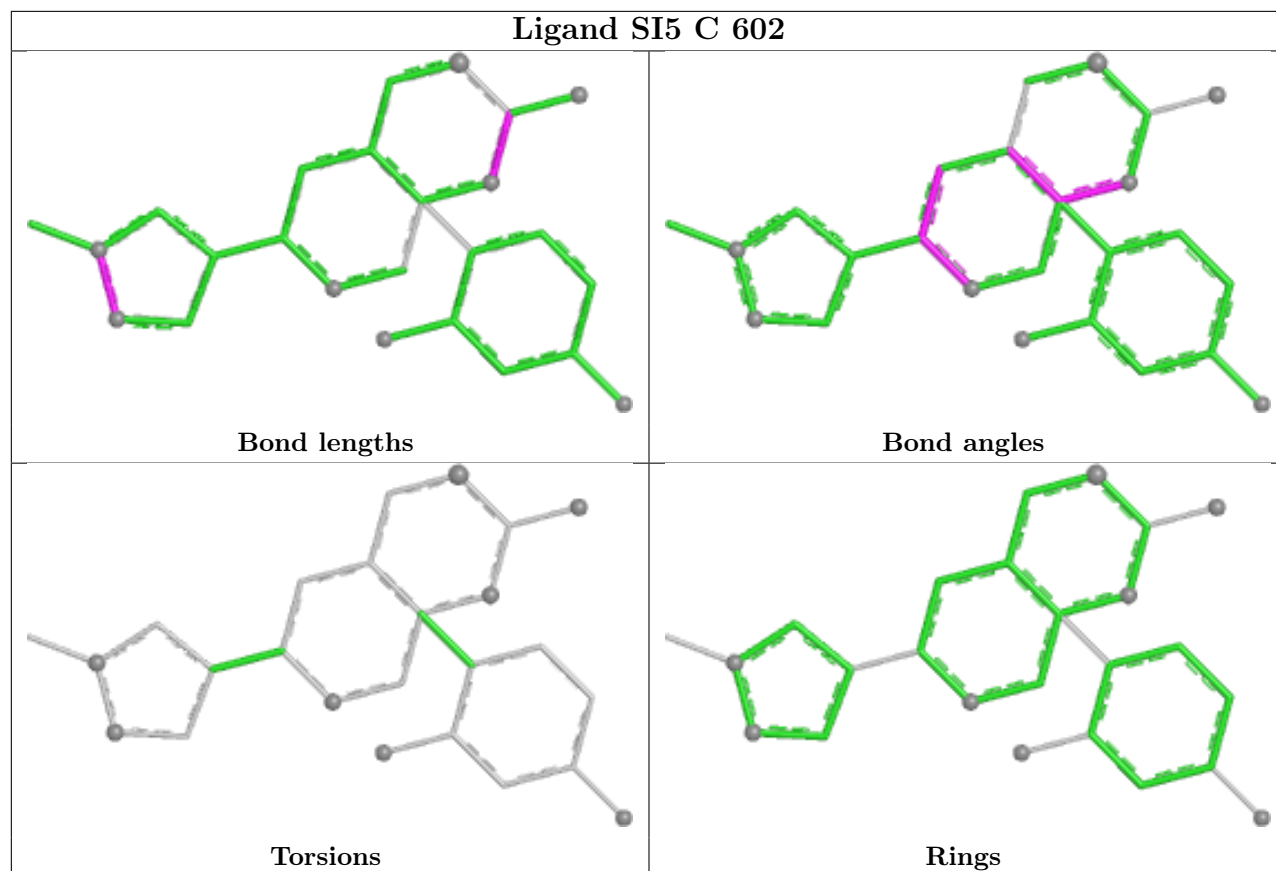
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

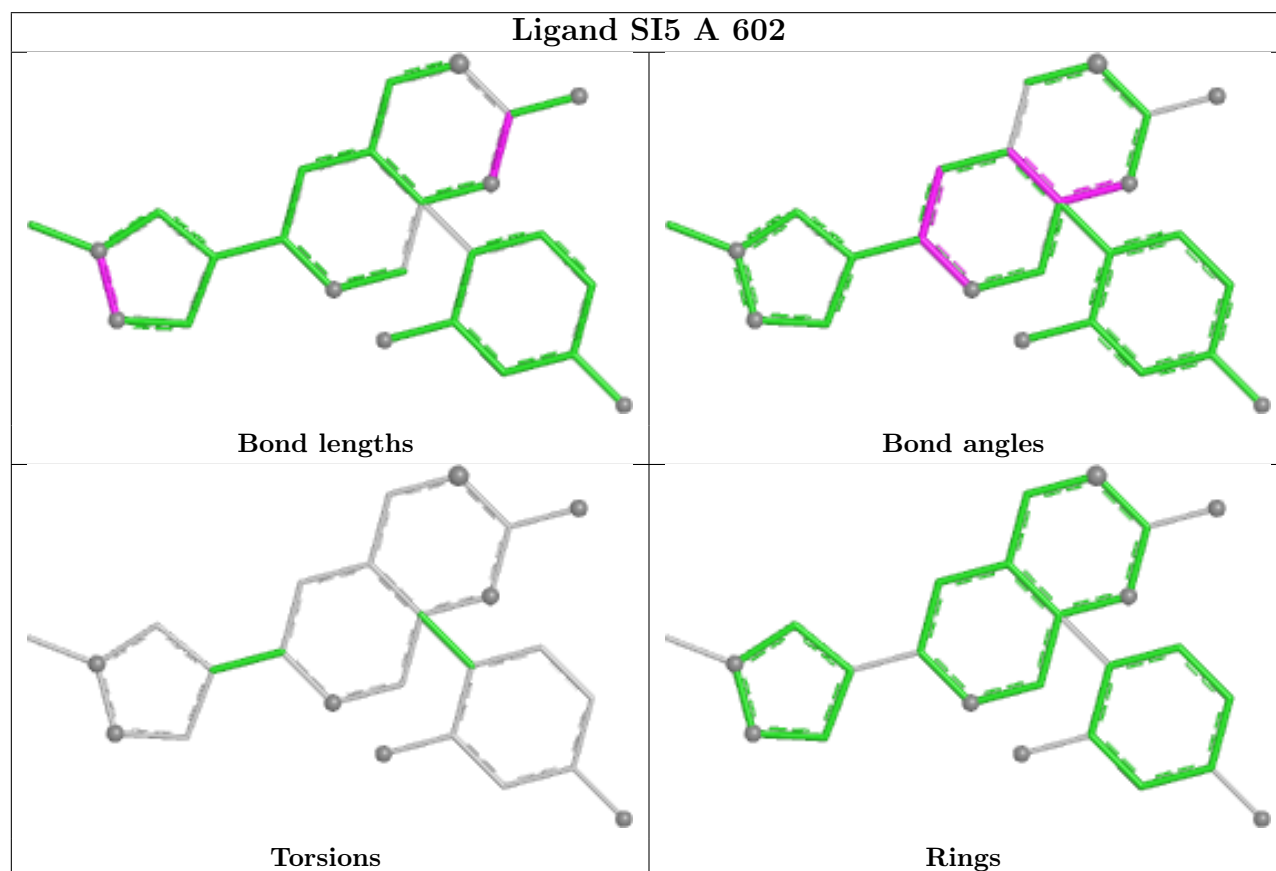


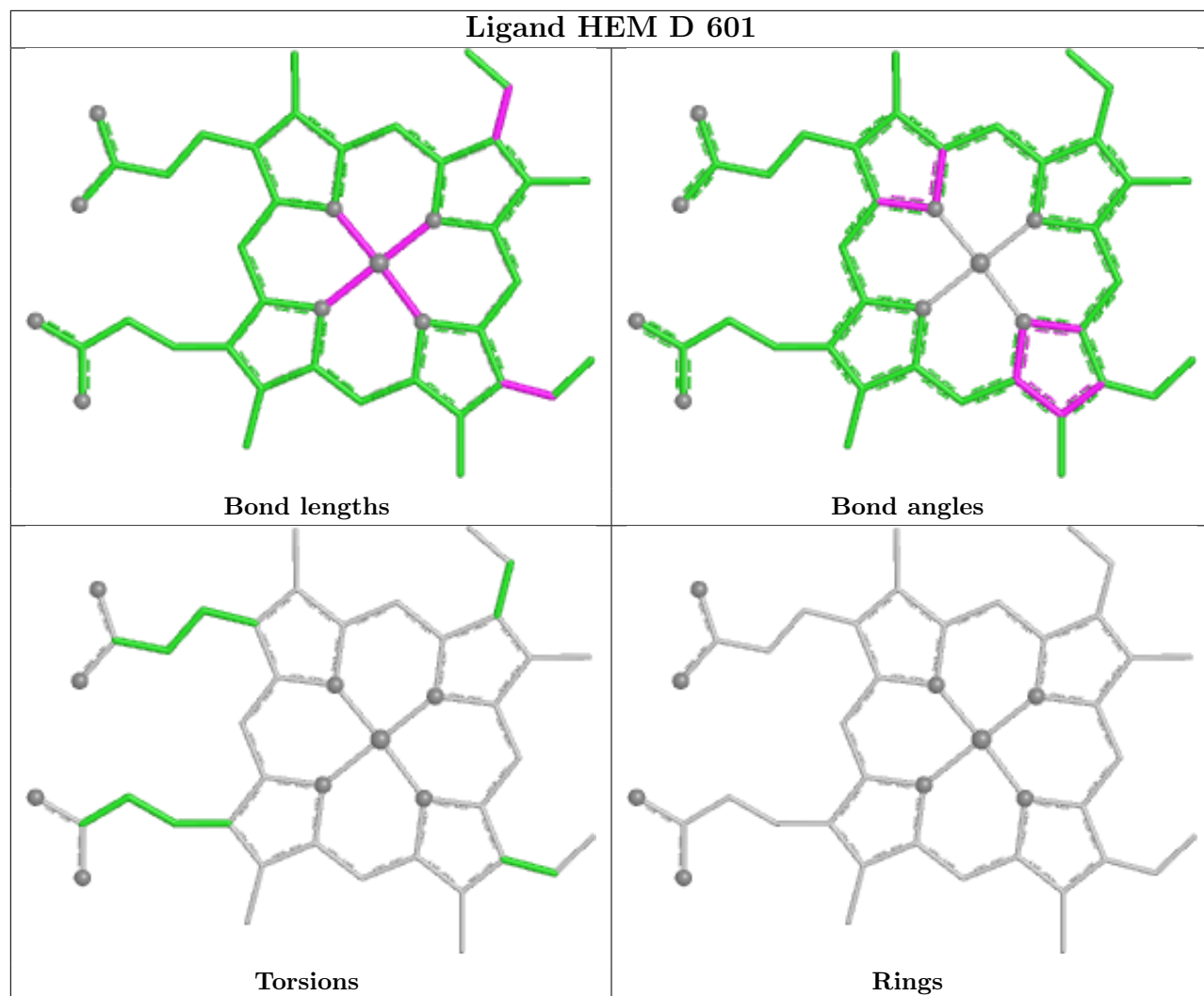


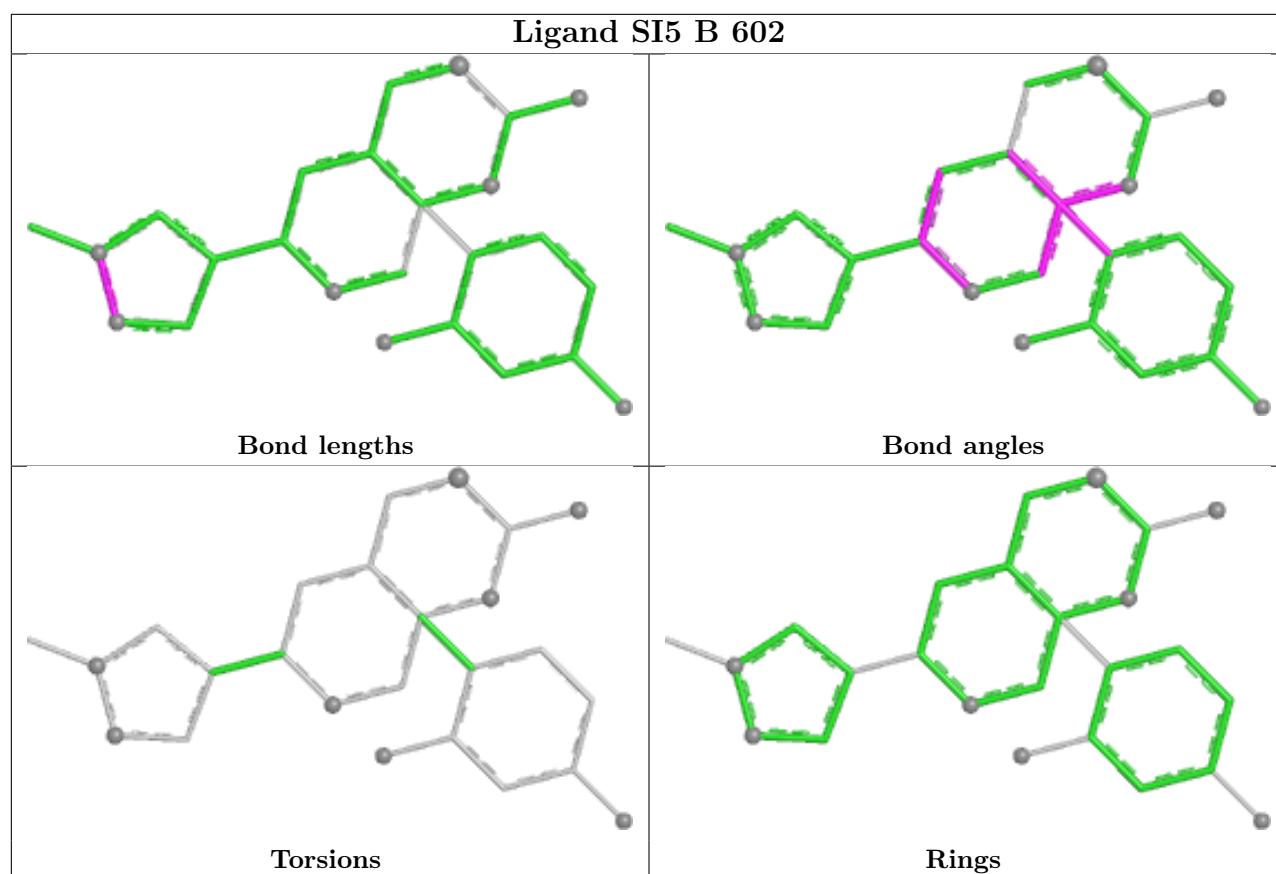
Ligand SI5 C 602

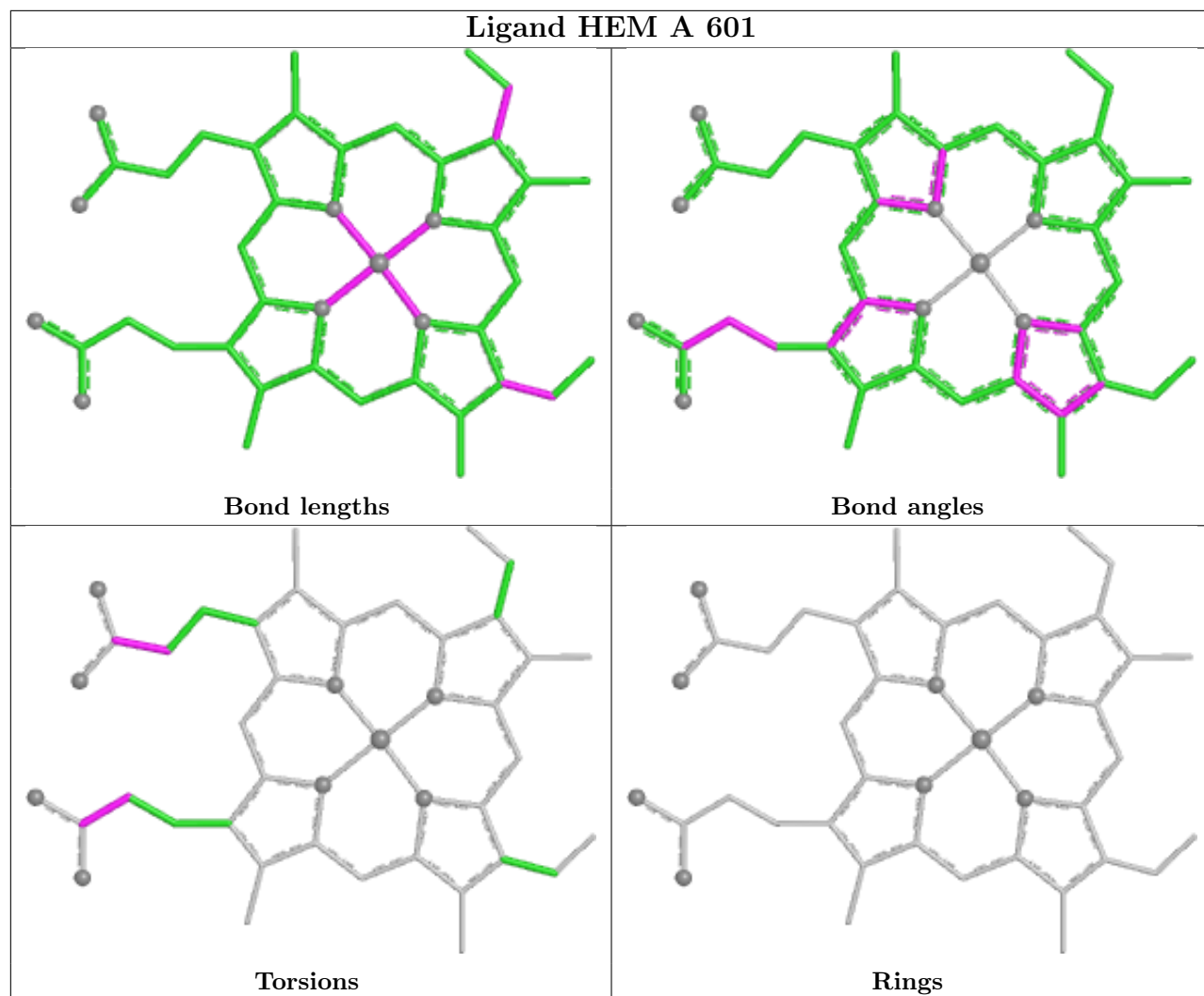


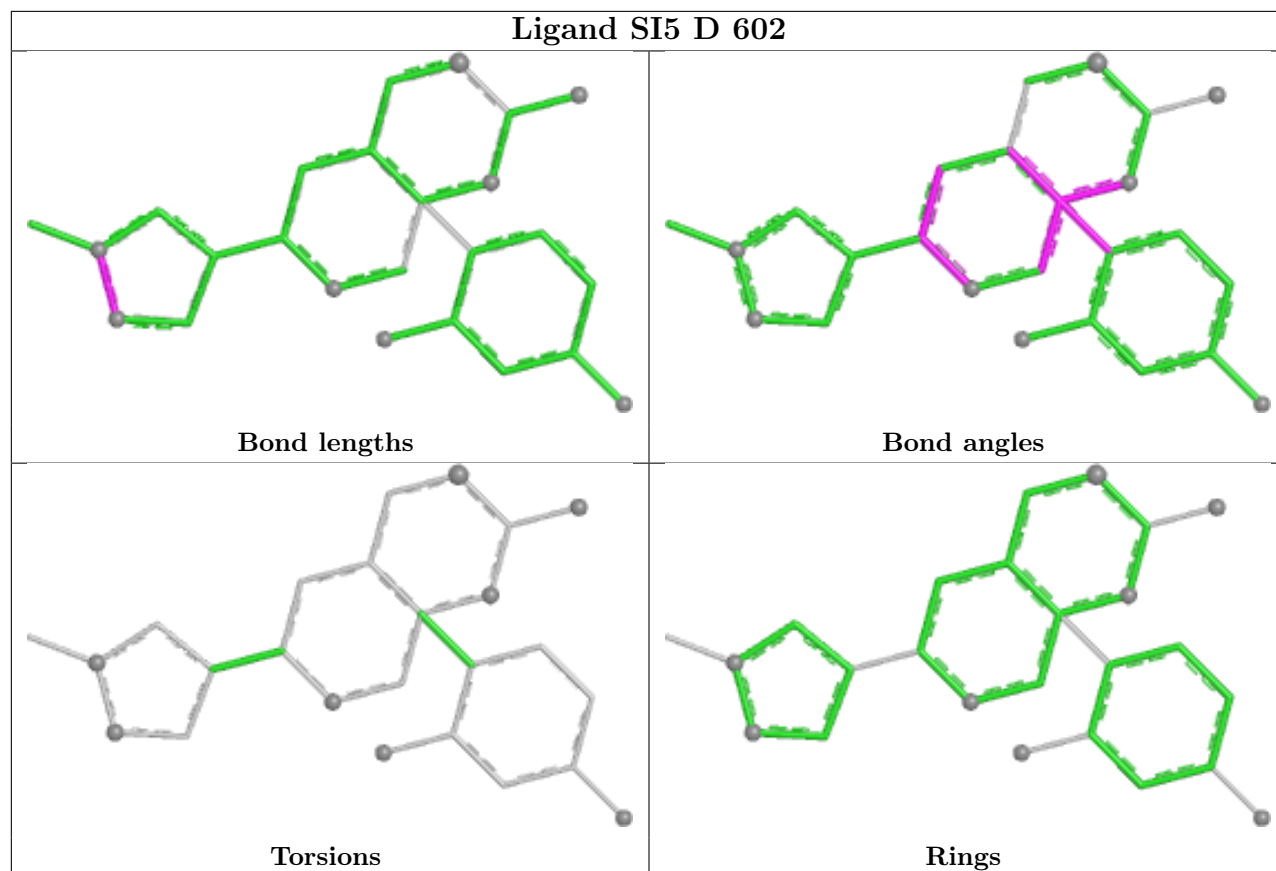
Ligand SI5 A 602











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	464/479 (96%)	0.52	49 (10%) 11 9	28, 47, 101, 124	0
1	B	455/479 (94%)	0.45	50 (10%) 10 8	26, 46, 100, 115	0
1	C	446/479 (93%)	0.67	50 (11%) 10 8	29, 52, 102, 123	0
1	D	452/479 (94%)	0.76	62 (13%) 6 5	31, 55, 104, 134	0
All	All	1817/1916 (94%)	0.60	211 (11%) 9 8	26, 50, 103, 134	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	TYR	5.7
1	D	75	TRP	5.7
1	B	219	PHE	5.4
1	B	149	LEU	5.4
1	A	75	TRP	5.1
1	B	39	PRO	5.0
1	C	39	PRO	4.9
1	D	40	LEU	4.7
1	A	38	LEU	4.6
1	A	483	PHE	4.5
1	C	149	LEU	4.4
1	C	56	TYR	4.4
1	A	149	LEU	4.3
1	C	481	PHE	4.3
1	C	152	TRP	4.3
1	A	219	PHE	4.3
1	A	144	LEU	4.2
1	D	426	HIS	4.2
1	D	219	PHE	4.2
1	C	38	LEU	4.1
1	A	47	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	149	LEU	4.0
1	B	49	VAL	4.0
1	B	48	HIS	3.9
1	C	148	SER	3.9
1	D	229	VAL	3.9
1	D	483	PHE	3.8
1	A	228	PRO	3.7
1	B	74	ALA	3.7
1	A	145	GLY	3.7
1	C	219	PHE	3.7
1	D	471	GLY	3.7
1	B	75	TRP	3.6
1	D	55	PRO	3.6
1	C	168	SER	3.6
1	B	44	GLY	3.6
1	D	481	PHE	3.6
1	B	229	VAL	3.6
1	C	239	LYS	3.6
1	B	148	SER	3.5
1	A	303	PHE	3.5
1	A	56	TYR	3.5
1	B	227	VAL	3.5
1	C	220	LEU	3.5
1	B	235	ALA	3.4
1	D	423	ALA	3.4
1	B	47	LEU	3.4
1	C	426	HIS	3.4
1	A	220	LEU	3.3
1	C	55	PRO	3.3
1	A	229	VAL	3.3
1	A	189	LEU	3.3
1	D	38	LEU	3.3
1	B	226	ALA	3.3
1	A	48	HIS	3.2
1	D	425	GLY	3.2
1	B	152	TRP	3.2
1	B	481	PHE	3.2
1	C	303	PHE	3.2
1	C	380	ARG	3.2
1	B	303	PHE	3.2
1	B	56	TYR	3.2
1	A	50	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	340	GLY	3.1
1	C	54	THR	3.1
1	C	482	ALA	3.1
1	A	32	LYS	3.1
1	B	38	LEU	3.1
1	B	341	GLN	3.1
1	C	33	LEU	3.1
1	C	224	LEU	3.1
1	C	471	GLY	3.1
1	D	227	VAL	3.1
1	A	40	LEU	3.0
1	C	483	PHE	3.0
1	B	106	ILE	3.0
1	D	220	LEU	3.0
1	B	233	ILE	3.0
1	A	235	ALA	3.0
1	A	481	PHE	3.0
1	D	235	ALA	2.9
1	A	39	PRO	2.9
1	D	58	PHE	2.9
1	A	307	MET	2.9
1	A	223	VAL	2.9
1	D	63	ARG	2.9
1	D	380	ARG	2.9
1	D	303	PHE	2.9
1	D	168	SER	2.9
1	A	342	VAL	2.9
1	C	142	LEU	2.9
1	D	231	LEU	2.9
1	C	480	VAL	2.8
1	A	226	ALA	2.8
1	A	482	ALA	2.8
1	D	230	LEU	2.8
1	B	142	LEU	2.8
1	B	189	LEU	2.8
1	C	342	VAL	2.8
1	D	74	ALA	2.8
1	D	106	ILE	2.7
1	B	482	ALA	2.7
1	C	425	GLY	2.7
1	A	233	ILE	2.7
1	D	109	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	75	TRP	2.7
1	D	189	LEU	2.7
1	B	223	VAL	2.7
1	B	342	VAL	2.7
1	A	236	LEU	2.7
1	C	423	ALA	2.7
1	B	483	PHE	2.7
1	D	133	ARG	2.7
1	D	482	ALA	2.7
1	C	223	VAL	2.6
1	A	143	GLY	2.6
1	B	239	LYS	2.6
1	C	65	PHE	2.6
1	D	146	LYS	2.6
1	D	228	PRO	2.6
1	B	213	LEU	2.6
1	D	152	TRP	2.5
1	A	74	ALA	2.5
1	B	212	GLY	2.5
1	D	59	ASP	2.5
1	A	148	SER	2.5
1	D	39	PRO	2.5
1	B	340	GLY	2.5
1	C	389	ILE	2.5
1	B	230	LEU	2.5
1	D	65	PHE	2.5
1	C	233	ILE	2.5
1	A	480	VAL	2.5
1	C	228	PRO	2.4
1	D	69	PHE	2.4
1	B	32	LYS	2.4
1	A	60	GLN	2.4
1	A	210	GLN	2.4
1	C	231	LEU	2.4
1	D	60	GLN	2.4
1	B	232	HIS	2.4
1	D	477	HIS	2.4
1	C	225	ASN	2.4
1	D	143	GLY	2.4
1	B	220	LEU	2.4
1	B	63	ARG	2.4
1	B	228	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	147	LYS	2.4
1	C	218	GLY	2.4
1	C	484	LEU	2.4
1	D	239	LYS	2.4
1	D	470	THR	2.3
1	A	31	GLY	2.3
1	D	233	ILE	2.3
1	D	421	LEU	2.3
1	B	240	VAL	2.3
1	B	379	SER	2.3
1	A	224	LEU	2.3
1	C	229	VAL	2.3
1	C	74	ALA	2.3
1	A	231	LEU	2.3
1	D	54	THR	2.2
1	B	304	SER	2.2
1	C	410	GLU	2.2
1	C	338	VAL	2.2
1	A	218	GLY	2.2
1	A	43	LEU	2.2
1	D	144	LEU	2.2
1	D	379	SER	2.2
1	D	389	ILE	2.2
1	A	96	GLU	2.2
1	C	235	ALA	2.2
1	A	239	LYS	2.2
1	D	232	HIS	2.2
1	D	352	HIS	2.2
1	D	484	LEU	2.2
1	B	58	PHE	2.2
1	D	37	PRO	2.2
1	D	240	VAL	2.2
1	D	225	ASN	2.2
1	D	307	MET	2.2
1	A	213	LEU	2.2
1	C	241	LEU	2.2
1	C	109	ILE	2.2
1	D	226	ALA	2.1
1	A	42	GLY	2.1
1	D	139	LEU	2.1
1	C	57	CYS	2.1
1	A	133	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	217	SER	2.1
1	C	388	ARG	2.1
1	A	46	LEU	2.1
1	B	54	THR	2.1
1	D	73	LEU	2.1
1	B	224	LEU	2.1
1	C	421	LEU	2.1
1	B	350	GLN	2.1
1	C	210	GLN	2.1
1	A	305	ALA	2.0
1	B	209	ALA	2.0
1	B	208	LEU	2.0
1	B	231	LEU	2.0
1	C	139	LEU	2.0
1	D	36	GLY	2.0
1	D	422	ASP	2.0
1	C	478	HIS	2.0
1	A	64	ARG	2.0
1	D	170	ARG	2.0
1	C	213	LEU	2.0
1	B	307	MET	2.0
1	B	217	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	D	607	1/1	0.74	0.13	130,130,130,130	0

Continued on next page...

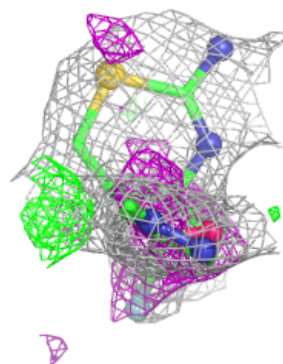
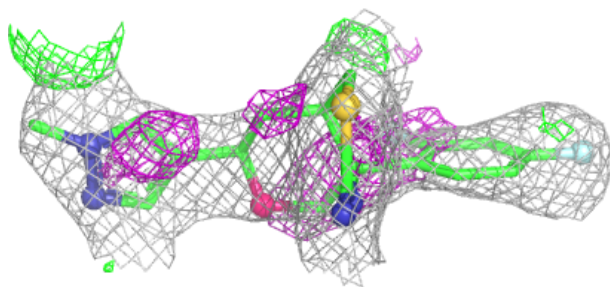
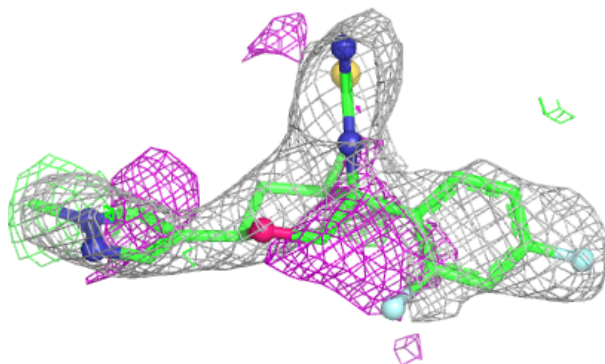
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	C	607	1/1	0.78	0.11	122,122,122,122	0
3	SI5	A	602	25/25	0.80	0.17	47,76,88,89	0
3	SI5	B	602	25/25	0.82	0.16	39,71,78,86	0
3	SI5	C	602	25/25	0.85	0.16	48,72,82,85	0
3	SI5	D	602	25/25	0.86	0.14	48,75,84,85	0
4	ZN	C	605	1/1	0.88	0.10	89,89,89,89	0
4	ZN	D	605	1/1	0.92	0.09	84,84,84,84	0
4	ZN	B	605	1/1	0.92	0.09	76,76,76,76	0
4	ZN	D	606	1/1	0.93	0.07	92,92,92,92	0
4	ZN	A	604	1/1	0.93	0.10	69,69,69,69	0
4	ZN	A	605	1/1	0.95	0.06	75,75,75,75	0
4	ZN	C	606	1/1	0.96	0.08	79,79,79,79	0
4	ZN	B	604	1/1	0.96	0.08	70,70,70,70	0
4	ZN	D	604	1/1	0.96	0.08	72,72,72,72	0
4	ZN	C	604	1/1	0.97	0.05	69,69,69,69	0
2	HEM	C	601	43/43	0.98	0.06	25,36,44,46	0
2	HEM	D	601	43/43	0.98	0.07	23,38,47,52	0
2	HEM	A	601	43/43	0.98	0.06	18,28,37,39	0
4	ZN	A	606	1/1	0.99	0.03	46,46,46,46	0
4	ZN	B	603	1/1	0.99	0.04	36,36,36,36	0
2	HEM	B	601	43/43	0.99	0.06	19,31,37,43	0
4	ZN	A	603	1/1	0.99	0.04	33,33,33,33	0
4	ZN	C	603	1/1	1.00	0.03	37,37,37,37	0
4	ZN	D	603	1/1	1.00	0.02	39,39,39,39	0

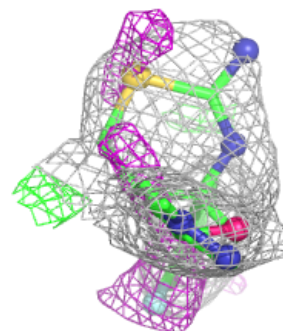
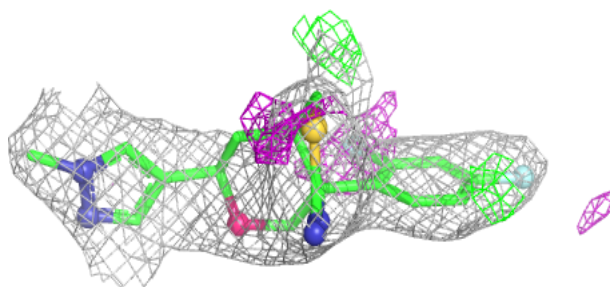
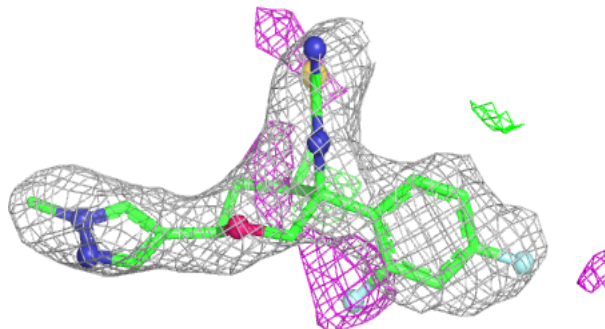
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SI5 A 602:

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

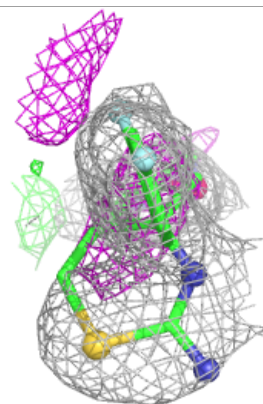
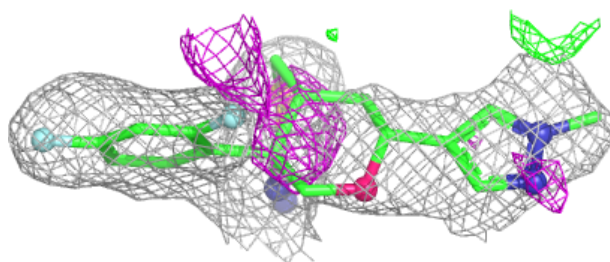
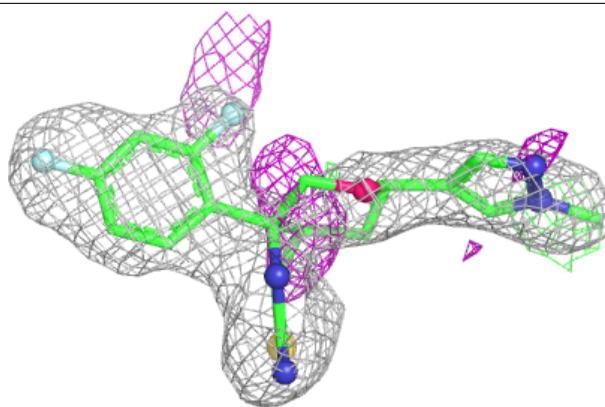
**Electron density around SI5 B 602:**

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

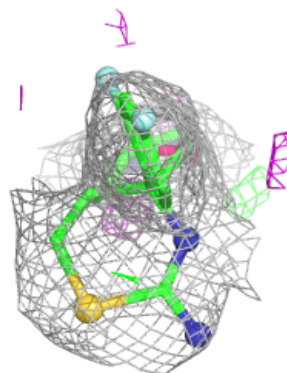
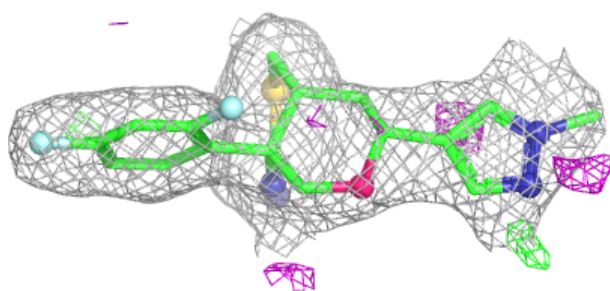
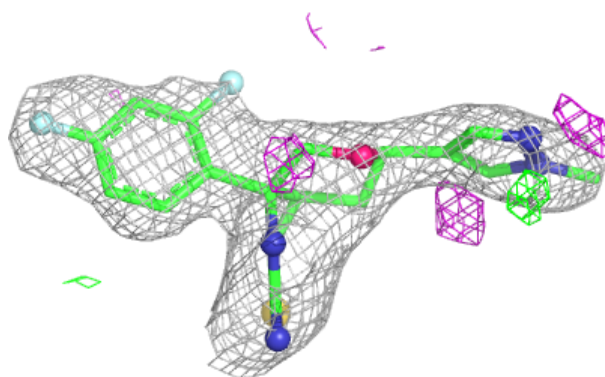


Electron density around SI5 C 602:

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

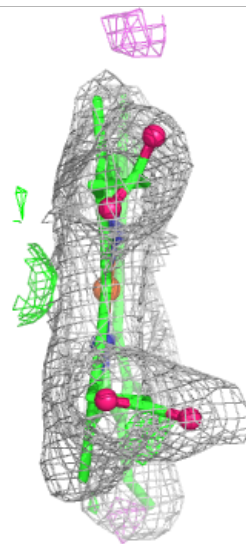
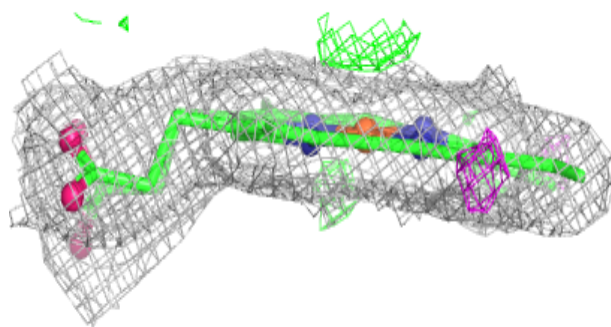
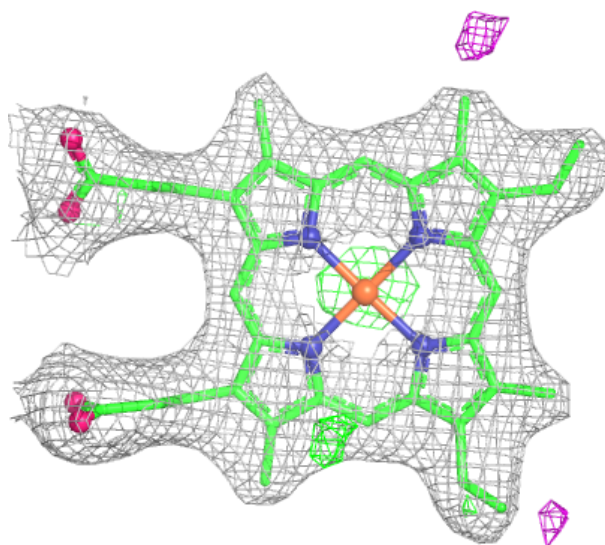
**Electron density around SI5 D 602:**

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



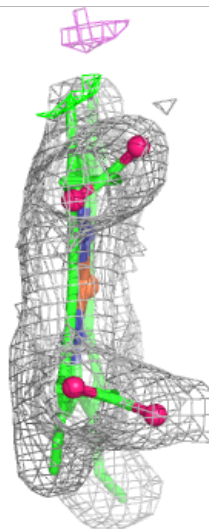
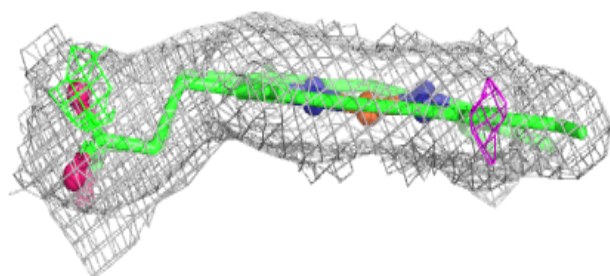
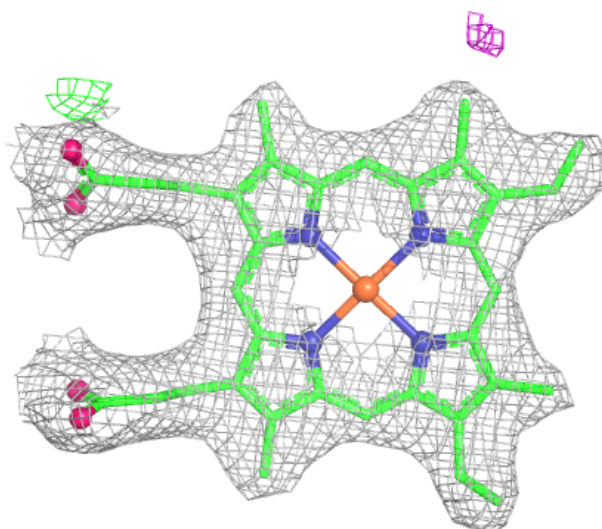
Electron density around HEM C 601:

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



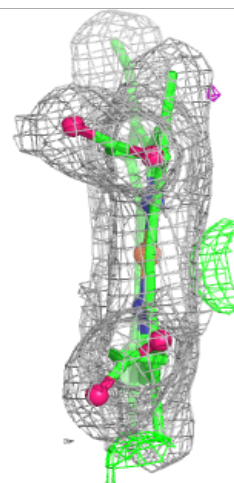
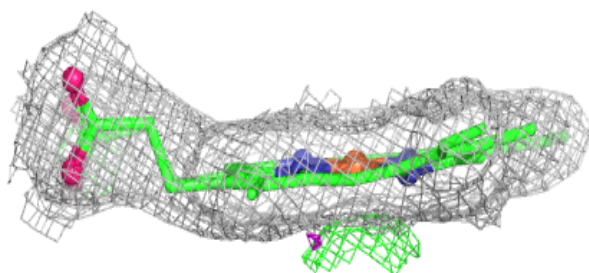
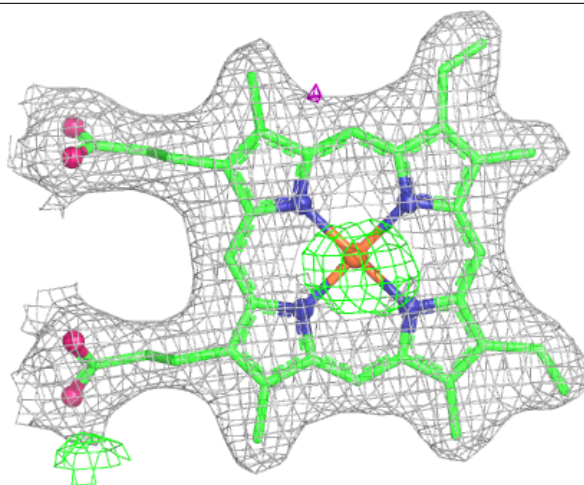
Electron density around HEM D 601:

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



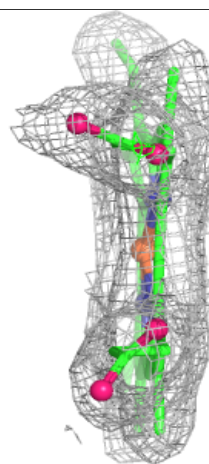
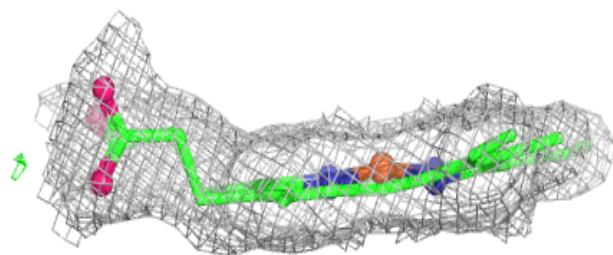
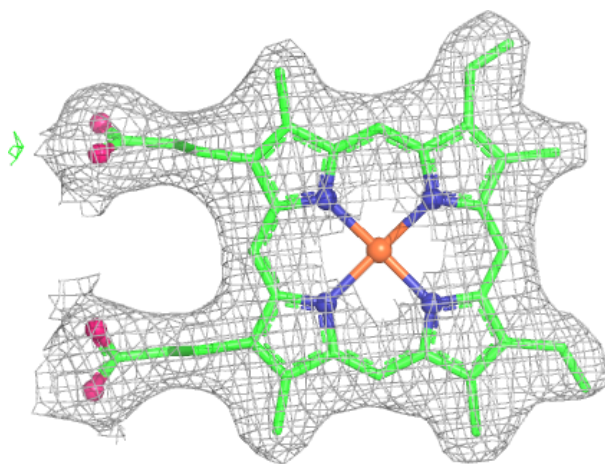
Electron density around HEM A 601:

$2mF_o-DF_c$ (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.