



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:47 PM UTC

PDB ID : 3N9Z / pdb_00003n9z
Title : Crystal structure of human CYP11A1 in complex with 22-hydroxycholesterol
Authors : Strushkevich, N.V.; MacKenzie, F.; Tempel, W.; Botchkarev, A.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.U.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2010-05-31
Resolution : 2.17 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

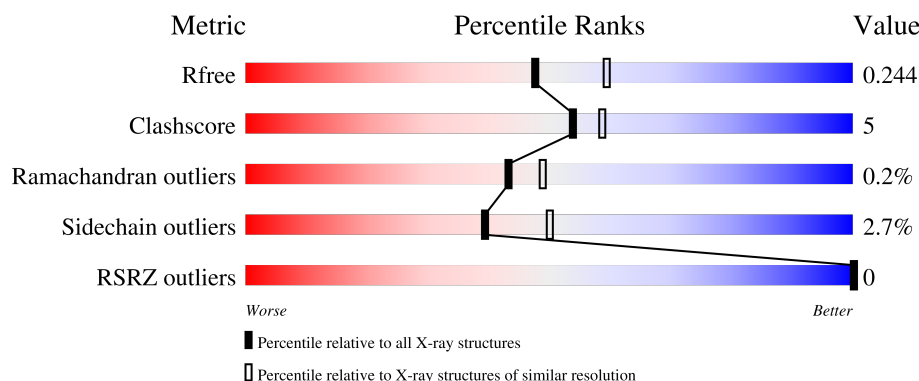
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	487	
1	B	487	
2	C	123	
2	D	123	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8772 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 Cholesterol side-chain cleavage enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3872	2511	666	679	16			
1	B	470	Total	C	N	O	S	0	0	0
			3872	2511	666	679	16			

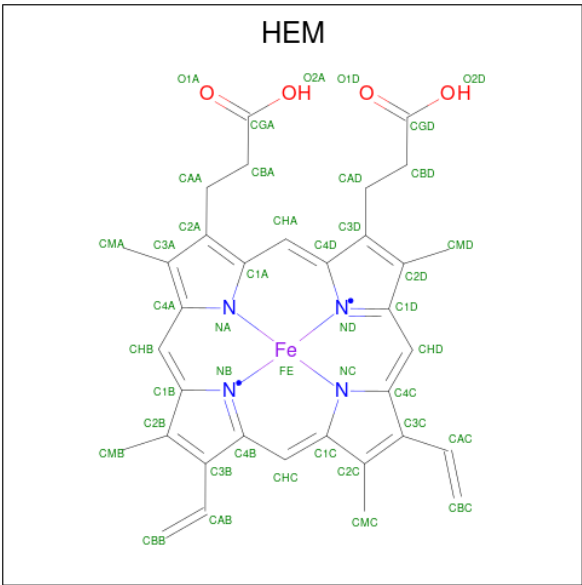
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	483	HIS	-	expression tag	UNP P05108
A	484	HIS	-	expression tag	UNP P05108
A	485	HIS	-	expression tag	UNP P05108
A	486	HIS	-	expression tag	UNP P05108
A	487	HIS	-	expression tag	UNP P05108
A	488	HIS	-	expression tag	UNP P05108
B	483	HIS	-	expression tag	UNP P05108
B	484	HIS	-	expression tag	UNP P05108
B	485	HIS	-	expression tag	UNP P05108
B	486	HIS	-	expression tag	UNP P05108
B	487	HIS	-	expression tag	UNP P05108
B	488	HIS	-	expression tag	UNP P05108

- Molecule 2 is a protein called Adrenodoxin.

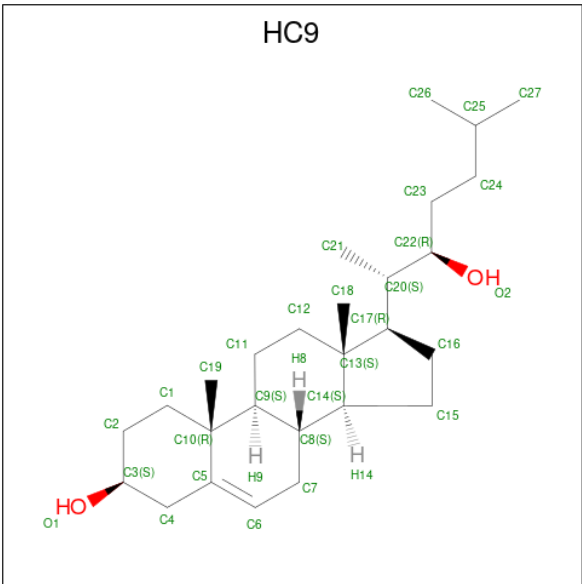
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	S	0	0	0
			194	113	33	43	5			
2	D	27	Total	C	N	O	S	0	0	0
			194	113	33	43	5			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is (3 α ,8 α ,22R)-cholest-5-ene-3,22-diol (CCD ID: HC9) (formula: C₂₇H₄₆O₂).



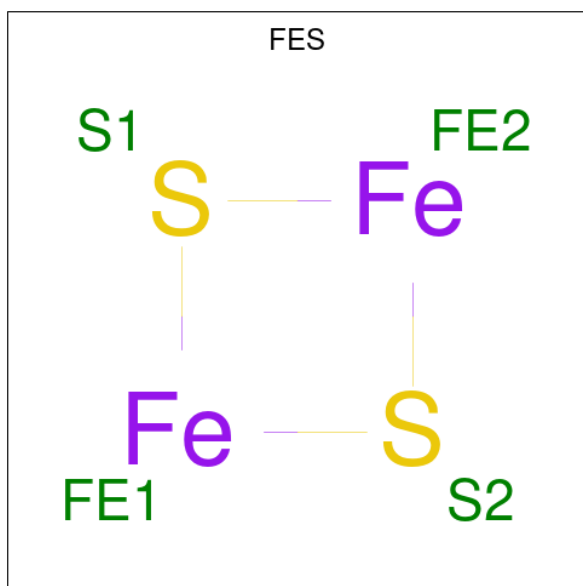
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	27	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			29	27	2		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

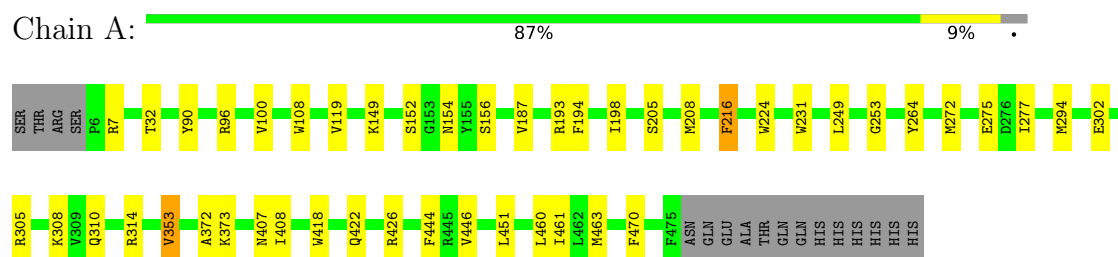
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	232	Total	O	0	0
			232	232		
6	B	252	Total	O	0	0
			252	252		
6	C	1	Total	O	0	0
			1	1		
6	D	3	Total	O	0	0
			3	3		

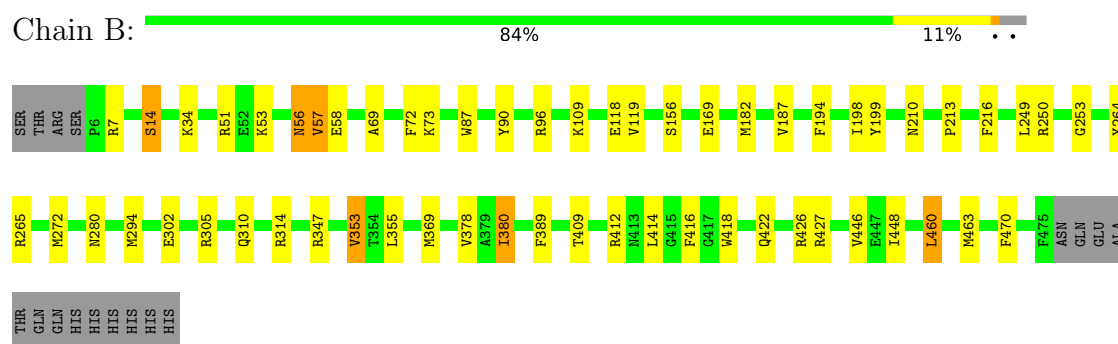
3 Residue-property plots

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

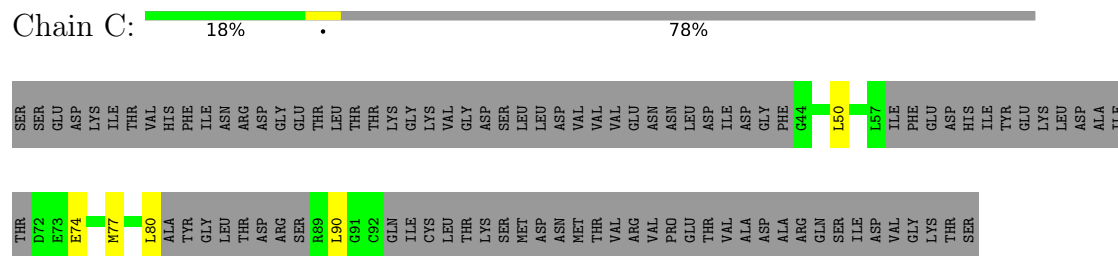
• Molecule 1: Cholesterol side-chain cleavage enzyme



• Molecule 1: Cholesterol side-chain cleavage enzyme



• Molecule 2: Adrenodoxin



• Molecule 2: Adrenodoxin



SER	SER	GLU	ASP	LYS	ILE	THR	VAL	HIS	PHE	ILE	ASN	ARG	ASP	GLY	GLU	THR	LEU	THR	THR	LYS	GLY	LYS	VAL	GLY	ASP	SER	ASN	LEU	LEU	ASP	VAL	VAL	VAL	GLU	ASN	ASN	LEU	ASP	ILE	ASP	GLY	PHE	G44	L57	ILE	PHE	GLU	GLU	ASP	HIS	ASP	ILE	TYR	GLU	LYS	LEU	ASP	ALA	ILE	THR	D72
E73	E74	M77	L80	ALA	TYR	GLY	LEU	THR	ASP	ARG	SER	R89	L90	G91	C92	GLN	ILE	CYS	LEU	THR	LYS	SER	MET	ASP	ASN	MET	THR	VAL	ARG	VAL	VAL	PRO	GLU	THR	VAL	ALA	ASP	ALA	ARG	GLN	SER	SER	ILE	ASP	VAL	GLY	LYS	THR	SER												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.38Å 115.09Å 86.21Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	20.00 – 2.17 20.00 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.17) 97.4 (20.00-2.17)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.17Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.210 , 0.243 0.211 , 0.244	Depositor DCC
R_{free} test set	4093 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.216 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8772	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: HC9, FES, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/3982	0.82	2/5403 (0.0%)
1	B	0.56	0/3982	0.81	2/5403 (0.0%)
2	C	0.51	0/192	0.80	0/254
2	D	0.47	0/192	0.73	0/254
All	All	0.56	0/8348	0.81	4/11314 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	VAL	CB-CA-C	-7.57	101.92	112.14
1	B	353	VAL	CB-CA-C	-6.66	101.84	112.16
1	B	57	VAL	N-CA-C	5.19	115.57	107.99
1	A	216	PHE	CB-CA-C	-5.11	100.25	110.42

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	3872	0	3842	33	0
1	B	3872	0	3842	42	0
2	C	194	0	171	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	194	0	171	4	0
3	A	43	0	30	1	0
3	B	43	0	30	0	0
4	A	29	0	46	0	0
4	B	29	0	46	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
6	A	232	0	0	3	0
6	B	252	0	0	5	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
All	All	8772	0	8178	80	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 5.

All (80) 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:208:MET:HE1	1:A:224:TRP:HB2	1.39	1.05
1:B:56:ASN:H	1:B:56:ASN:HD22	1.05	0.93
1:B:57:VAL:HG12	6:B:575:HOH:O	1.69	0.90
1:A:310:GLN:HE21	1:A:314:ARG:HH22	1.18	0.86
1:B:310:GLN:HE21	1:B:314:ARG:HH22	1.22	0.85
1:A:208:MET:CE	1:A:224:TRP:HB2	2.10	0.82
1:B:310:GLN:HE22	1:B:446:VAL:H	1.31	0.78
1:B:56:ASN:H	1:B:56:ASN:ND2	1.81	0.77
1:A:310:GLN:HE22	1:A:446:VAL:H	1.30	0.77
1:A:194:PHE:CE2	1:A:198:ILE:HD11	2.21	0.76
1:B:294:MET:HA	1:B:294:MET:HE2	1.68	0.74
1:A:418:TRP:HD1	2:C:80:LEU:HD23	1.51	0.74
1:B:210:ASN:HA	6:B:575:HOH:O	1.87	0.73
1:A:205:SER:CB	1:A:460:LEU:HD12	2.19	0.73
1:B:194:PHE:CE2	1:B:198:ILE:HD11	2.28	0.69
1:B:418:TRP:HE1	2:D:80:LEU:HB3	1.59	0.68
1:B:199:TYR:HE1	1:B:463:MET:HE1	1.58	0.68
1:B:69:ALA:O	1:B:73:LYS:HG2	1.95	0.67
1:B:56:ASN:HD22	1:B:56:ASN:N	1.84	0.67
1:A:461:ILE:HD11	1:A:463:MET:HE3	1.75	0.67
1:B:272:MET:HE1	1:B:280:ASN:HD22	1.60	0.66
1:A:294:MET:HA	1:A:294:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:PHE:O	1:B:412:ARG:NH1	2.30	0.65
1:A:205:SER:HB2	1:A:460:LEU:HD12	1.79	0.64
1:A:208:MET:HE2	1:A:216:PHE:HB3	1.81	0.62
2:C:74:GLU:HG3	2:C:90:LEU:HD12	1.82	0.61
3:A:601:HEM:HBB2	3:A:601:HEM:HMB2	1.83	0.60
1:B:378:VAL:HG12	1:B:380:ILE:HD12	1.84	0.59
1:B:422:GLN:NE2	1:B:426:ARG:HH11	2.02	0.57
2:C:77:MET:HA	2:C:77:MET:HE2	1.86	0.56
1:A:208:MET:CE	1:A:216:PHE:HB3	2.38	0.54
2:D:74:GLU:HG3	2:D:90:LEU:HD12	1.90	0.54
1:B:427:ARG:HD2	6:B:550:HOH:O	2.07	0.53
1:B:272:MET:HE1	1:B:280:ASN:ND2	2.24	0.52
1:B:14:SER:HB2	1:B:51:ARG:O	2.09	0.51
1:B:418:TRP:CD1	2:D:80:LEU:HD13	2.45	0.51
1:B:355:LEU:HG	1:B:380:ILE:HD13	1.92	0.51
1:A:305:ARG:HG2	1:A:451:LEU:HD21	1.92	0.51
1:A:310:GLN:NE2	1:A:314:ARG:HH22	1.98	0.51
1:B:422:GLN:HE21	1:B:426:ARG:HD2	1.76	0.50
1:A:422:GLN:HE21	1:A:426:ARG:HD2	1.77	0.49
1:A:193:ARG:NH2	6:A:665:HOH:O	2.46	0.49
1:B:109:LYS:NZ	6:B:656:HOH:O	2.47	0.47
1:A:208:MET:HE2	1:A:216:PHE:CB	2.44	0.47
1:A:314:ARG:NH2	1:A:444:PHE:O	2.48	0.46
1:B:156:SER:HA	1:B:470:PHE:O	2.15	0.46
1:B:169:GLU:HG2	1:B:182:MET:HB2	1.97	0.46
1:A:208:MET:HE1	1:A:224:TRP:CB	2.27	0.46
1:A:154:ASN:ND2	6:A:668:HOH:O	2.44	0.46
1:A:205:SER:HB3	1:A:460:LEU:HD12	1.94	0.46
1:A:272:MET:HB3	1:A:277:ILE:HG13	1.97	0.46
1:B:310:GLN:NE2	1:B:314:ARG:HH22	2.03	0.45
2:D:77:MET:HE2	2:D:77:MET:HA	1.99	0.45
1:A:302:GLU:OE2	1:A:305:ARG:NH1	2.50	0.45
1:A:422:GLN:NE2	1:A:426:ARG:HH11	2.15	0.44
1:B:87:TRP:CZ2	1:B:460:LEU:HD22	2.53	0.44
1:B:294:MET:HA	1:B:294:MET:CE	2.44	0.44
1:B:422:GLN:NE2	1:B:426:ARG:HD2	2.33	0.44
1:A:100:VAL:HG22	1:A:108:TRP:CD1	2.53	0.43
1:A:422:GLN:NE2	1:A:426:ARG:HD2	2.33	0.43
1:A:156:SER:HA	1:A:470:PHE:O	2.19	0.43
1:A:372:ALA:O	1:A:373:LYS:HB2	2.19	0.43
1:B:118:GLU:OE1	1:B:265:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:CZ	1:A:231:TRP:HB3	2.54	0.42
1:B:302:GLU:OE2	1:B:305:ARG:NH1	2.52	0.41
1:B:34:LYS:HE2	6:B:638:HOH:O	2.20	0.41
1:B:272:MET:CE	1:B:280:ASN:HD22	2.30	0.41
1:B:409:THR:HA	1:B:412:ARG:HG3	2.03	0.41
1:A:96:ARG:NH1	6:A:616:HOH:O	2.53	0.41
1:A:152:SER:OG	1:A:154:ASN:HB3	2.21	0.41
1:A:249:LEU:HD11	1:A:264:TYR:CD1	2.55	0.41
1:B:213:PRO:HA	1:B:216:PHE:CZ	2.55	0.41
1:B:249:LEU:HD11	1:B:264:TYR:CD1	2.55	0.41
1:B:53:LYS:HA	1:B:58:GLU:HA	2.02	0.41
1:B:90:TYR:CE2	1:B:96:ARG:HG3	2.56	0.41
1:A:90:TYR:CE2	1:A:231:TRP:HB3	2.56	0.41
1:B:72:PHE:HB3	1:B:418:TRP:CZ3	2.56	0.41
1:B:416:PHE:CG	1:B:426:ARG:HG3	2.56	0.40
1:B:310:GLN:NE2	1:B:446:VAL:H	2.09	0.40
1:B:380:ILE:HD11	1:B:414:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/487 (96%)	455 (97%)	12 (3%)	1 (0%)	43	49
1	B	468/487 (96%)	456 (97%)	11 (2%)	1 (0%)	43	49
2	C	21/123 (17%)	17 (81%)	4 (19%)	0	100	100
2	D	21/123 (17%)	19 (90%)	2 (10%)	0	100	100
All	All	978/1220 (80%)	947 (97%)	29 (3%)	2 (0%)	43	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	GLY
1	A	253	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/434 (96%)	408 (98%)	10 (2%)	43	55
1	B	418/434 (96%)	406 (97%)	12 (3%)	37	47
2	C	22/108 (20%)	21 (96%)	1 (4%)	24	30
2	D	22/108 (20%)	21 (96%)	1 (4%)	24	30
All	All	880/1084 (81%)	856 (97%)	24 (3%)	39	50

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	32	THR
1	A	119	VAL
1	A	149	LYS
1	A	187	VAL
1	A	275	GLU
1	A	308	LYS
1	A	353	VAL
1	A	407	ASN
1	A	408	ILE
1	B	7	ARG
1	B	14	SER
1	B	56	ASN
1	B	119	VAL
1	B	187	VAL
1	B	250	ARG
1	B	347	ARG
1	B	353	VAL
1	B	369	MET
1	B	380	ILE

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Mol	Chain	Res	Type
1	B	448	ILE
1	B	460	LEU
2	C	50	LEU
2	D	92	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	154	ASN
1	A	299	HIS
1	A	310	GLN
1	A	422	GLN
1	A	450	HIS
1	B	56	ASN
1	B	78	ASN
1	B	299	HIS
1	B	310	GLN
1	B	422	GLN
1	B	449	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 [i](#)

6 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
5	FES	D	151	2	0,4,4	-	-	-		
3	HEM	A	601	1,4	50,50,50	1.97	9 (18%)	67,82,82	1.37	8 (11%)
3	HEM	B	601	1,4	50,50,50	1.96	9 (18%)	67,82,82	1.32	5 (7%)
4	HC9	A	602	3	32,32,32	0.49	0	50,50,50	1.12	4 (8%)
5	FES	C	150	2	0,4,4	-	-	-		
4	HC9	B	602	3	32,32,32	0.50	0	50,50,50	0.91	2 (4%)

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
5	FES	D	151	2	-	-	0/1/1/1
3	HEM	A	601	1,4	-	2/14/54/54	-
3	HEM	B	601	1,4	-	2/14/54/54	-
4	HC9	A	602	3	-	3/13/71/71	0/4/4/4
5	FES	C	150	2	-	-	0/1/1/1
4	HC9	B	602	3	-	1/13/71/71	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	HEM	C3D-C2D	7.66	1.53	1.36
3	A	601	HEM	C3D-C2D	7.54	1.53	1.36
3	A	601	HEM	FE-ND	5.78	2.12	1.94
3	B	601	HEM	FE-ND	4.85	2.09	1.94
3	A	601	HEM	FE-NB	4.27	2.08	1.94
3	B	601	HEM	FE-NB	4.16	2.07	1.94
3	A	601	HEM	FE-NC	4.04	2.08	1.95
3	B	601	HEM	FE-NC	3.83	2.07	1.95
3	B	601	HEM	FE-NA	3.44	2.06	1.95
3	A	601	HEM	CAB-C3B	3.14	1.55	1.47
3	B	601	HEM	CAB-C3B	3.10	1.55	1.47
3	B	601	HEM	CAC-C3C	2.76	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	HEM	CMC-C2C	2.62	1.56	1.50
3	A	601	HEM	CAC-C3C	2.52	1.54	1.47
3	A	601	HEM	CMC-C2C	2.47	1.55	1.50
3	B	601	HEM	CMB-C2B	2.46	1.55	1.50
3	A	601	HEM	CMD-C2D	2.32	1.55	1.50
3	A	601	HEM	CMB-C2B	2.24	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	HEM	C4D-ND-C1D	5.58	111.82	105.21
3	A	601	HEM	C4D-ND-C1D	5.43	111.64	105.21
4	A	602	HC9	C4-C5-C10	3.32	120.68	116.42
4	B	602	HC9	C4-C5-C10	2.77	119.97	116.42
3	A	601	HEM	C4C-C3C-C2C	2.57	109.04	106.81
4	A	602	HC9	C4-C5-C6	-2.44	117.26	120.57
3	B	601	HEM	CBD-CAD-C3D	-2.40	105.90	112.53
4	B	602	HC9	C4-C5-C6	-2.40	117.32	120.57
3	A	601	HEM	C1B-NB-C4B	2.38	108.02	105.21
3	A	601	HEM	C2A-C1A-NA	-2.36	107.53	110.15
3	A	601	HEM	CBD-CAD-C3D	-2.36	106.01	112.53
4	A	602	HC9	C7-C8-C9	-2.31	107.05	109.72
3	B	601	HEM	C1B-NB-C4B	2.25	107.87	105.21
3	A	601	HEM	CMD-C2D-C1D	2.15	128.39	125.03
3	A	601	HEM	CBA-CAA-C2A	-2.10	106.72	112.53
3	A	601	HEM	O2D-CGD-CBD	2.06	120.50	114.00
4	A	602	HC9	C19-C10-C9	-2.02	109.39	111.66
3	B	601	HEM	CAD-C3D-C4D	2.01	128.20	124.70
3	B	601	HEM	C4C-C3C-C2C	2.01	108.56	106.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

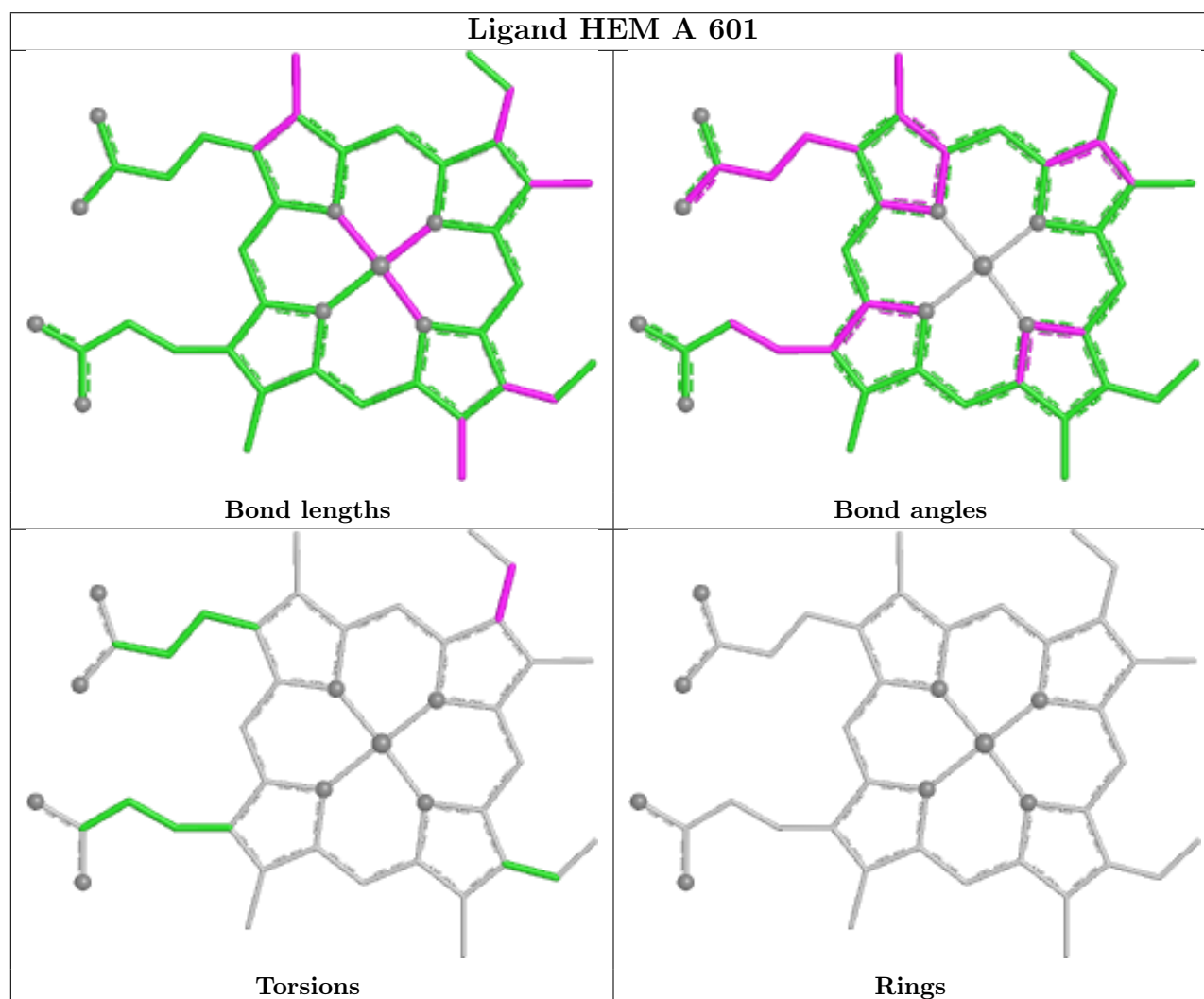
Mol	Chain	Res	Type	Atoms
3	A	601	HEM	C2C-C3C-CAC-CBC
3	B	601	HEM	C2C-C3C-CAC-CBC
3	B	601	HEM	C4C-C3C-CAC-CBC
4	B	602	HC9	C22-C23-C24-C25
3	A	601	HEM	C4C-C3C-CAC-CBC
4	A	602	HC9	O2-C22-C23-C24
4	A	602	HC9	C20-C22-C23-C24
4	A	602	HC9	C22-C23-C24-C25

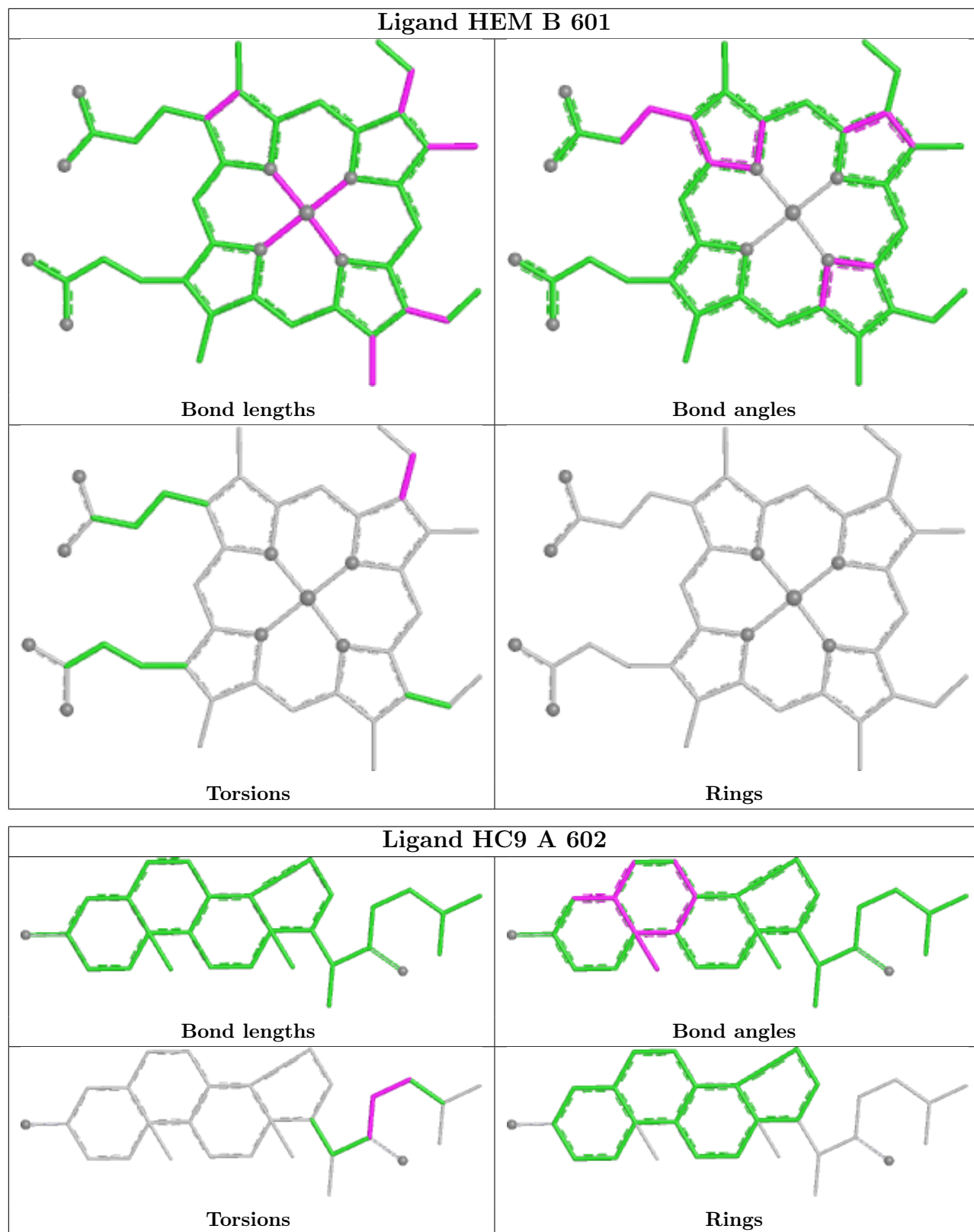
There are no ring outliers.

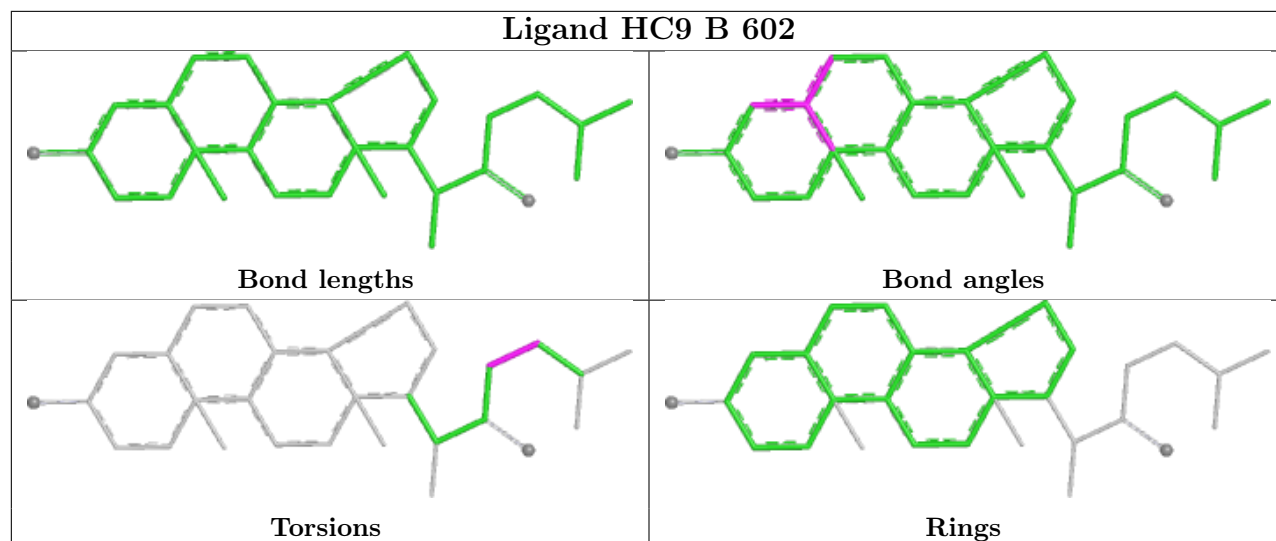
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	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.







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	470/487 (96%)	-1.50	0 100 100	13, 23, 37, 48	0
1	B	470/487 (96%)	-1.49	0 100 100	12, 24, 39, 49	0
2	C	27/123 (21%)	-0.70	0 100 100	60, 67, 74, 75	0
2	D	27/123 (21%)	-0.53	0 100 100	64, 72, 74, 74	0
All	All	994/1220 (81%)	-1.45	0 100 100	12, 24, 61, 75	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.

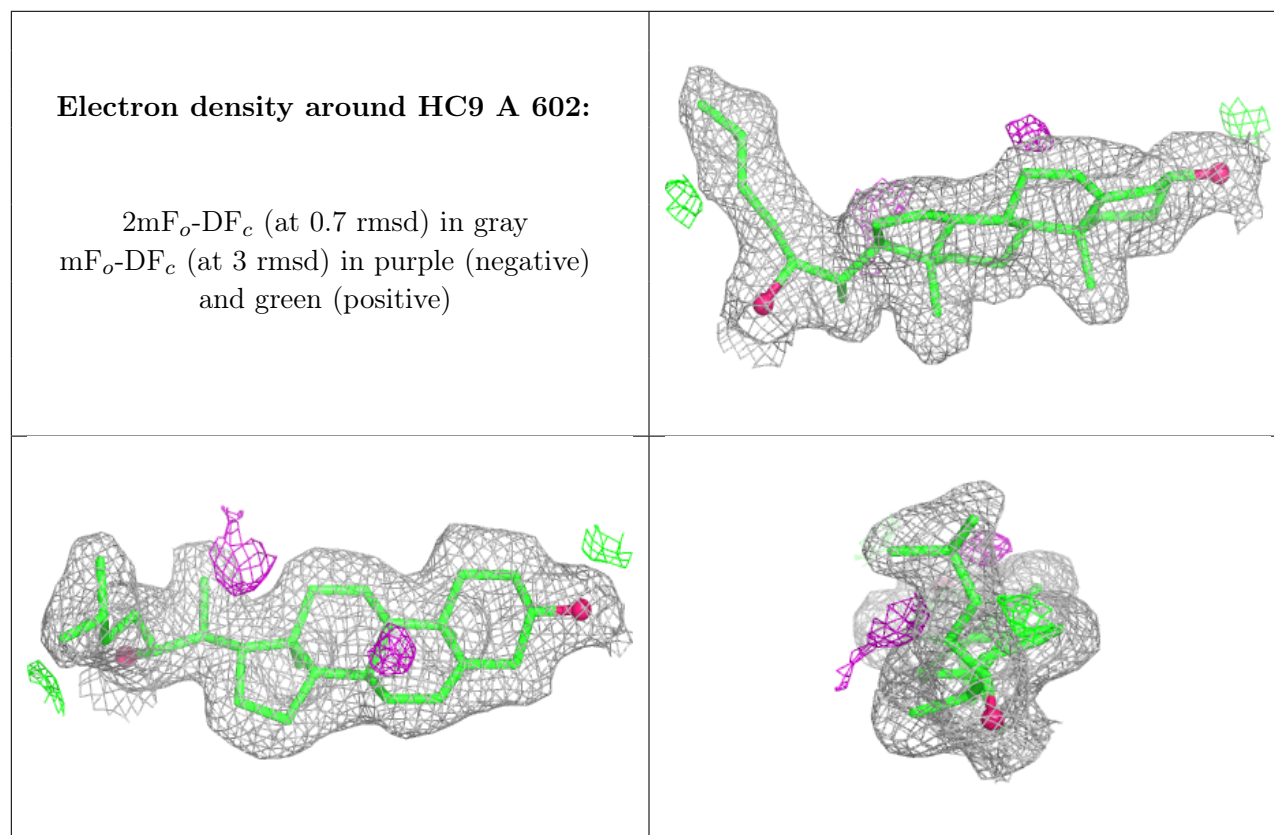
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HC9	A	602	29/29	0.99	0.03	12,14,25,27	0
4	HC9	B	602	29/29	0.99	0.02	10,12,25,26	0
5	FES	C	150	4/4	0.99	0.05	59,60,60,61	0
5	FES	D	151	4/4	0.99	0.06	61,61,62,63	0

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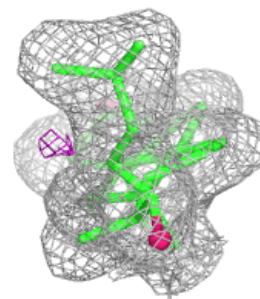
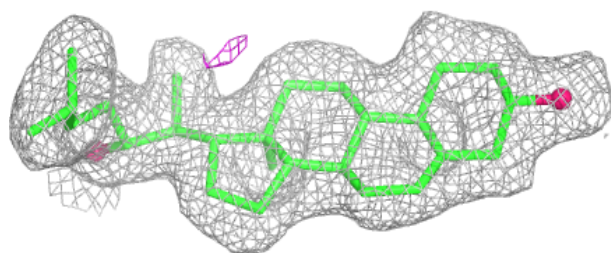
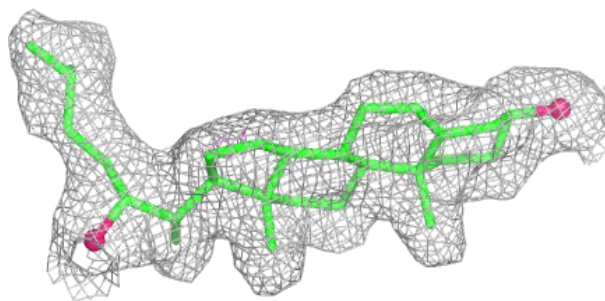
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	A	601	43/43	1.00	0.02	9,14,15,17	0
3	HEM	B	601	43/43	1.00	0.02	10,14,15,18	0

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.



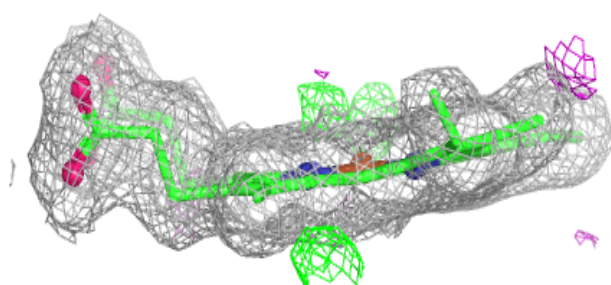
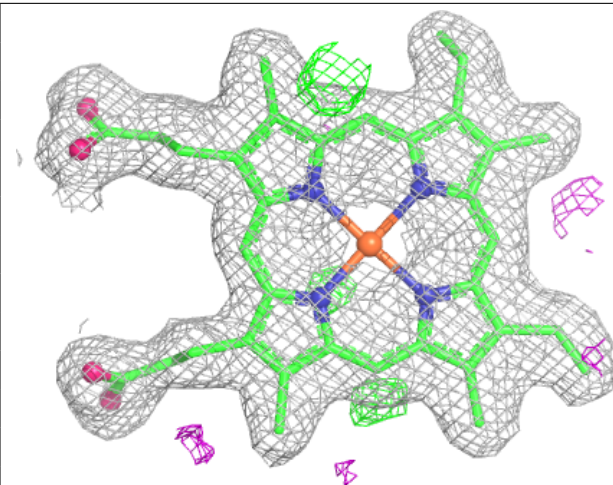
Electron density around HC9 B 602:

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



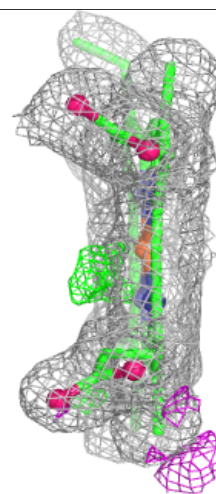
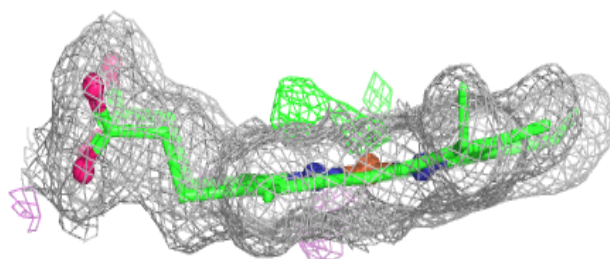
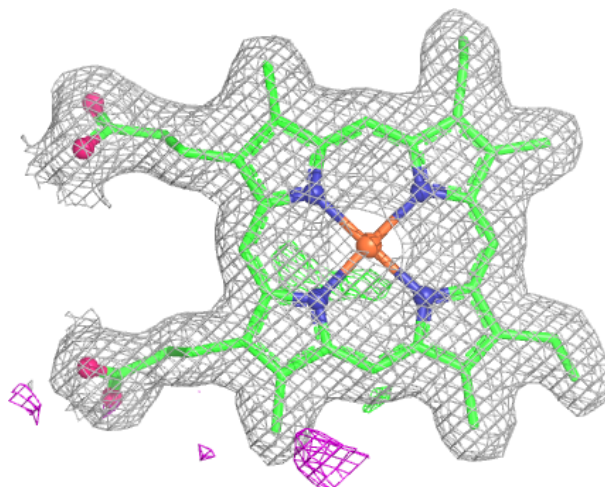
Electron density around HEM A 601:

$2mF_o-DF_c$ (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.