



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2022 – 02:10 PM JST

PDB ID : 7F3H  
Title : Crystal structure of cytochrome P450DA heme domain  
Authors : Wan, N.W.  
Deposited on : 2021-06-16  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

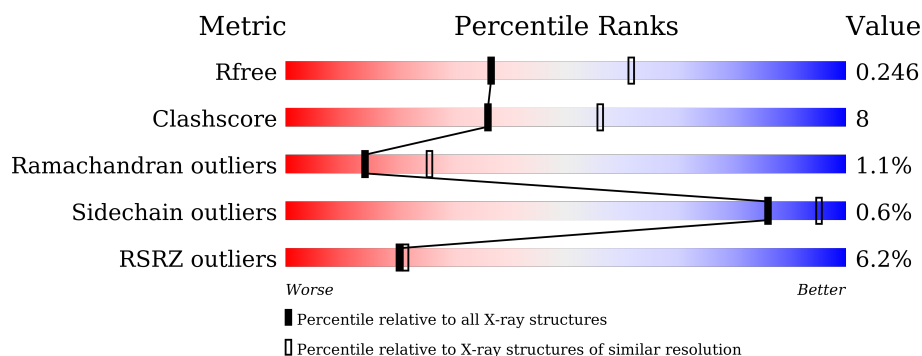
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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  $\geq 3$ , 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	501	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	501	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>• 9%</div> </div> </div>
1	C	501	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>• 10%</div> </div> </div>
1	D	501	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div> </div>

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

ria:

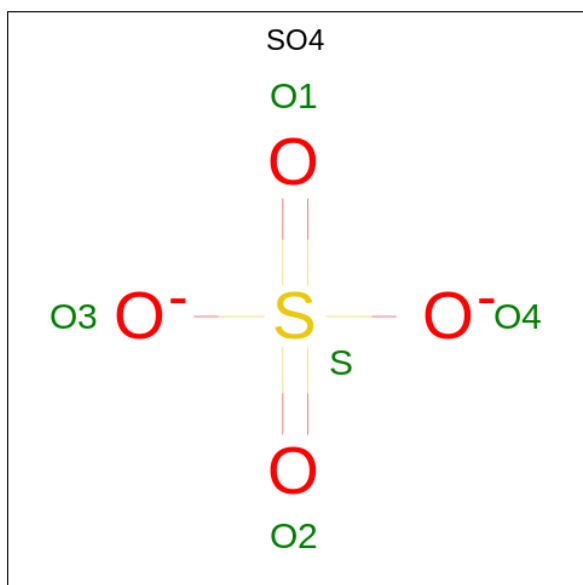
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SER	B	601	-	-	-	X



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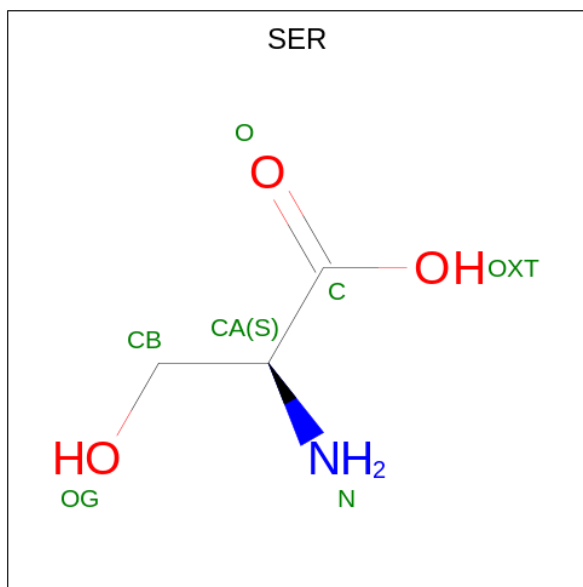
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S		
			5	4	1	0	0
3	A	1	Total	O	S		
			5	4	1	0	0
3	D	1	Total	O	S		
			5	4	1	0	0

- Molecule 4 is SERINE (three-letter code: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			6	3	1	2		

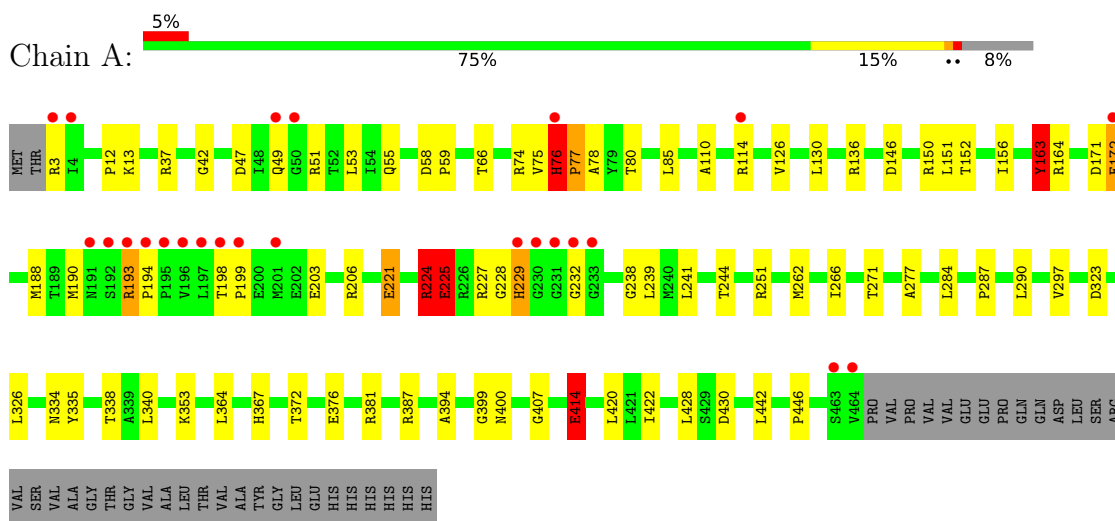
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	69	Total	O	0	0
			69	69		
5	C	55	Total	O	0	0
			55	55		
5	D	65	Total	O	0	0
			65	65		

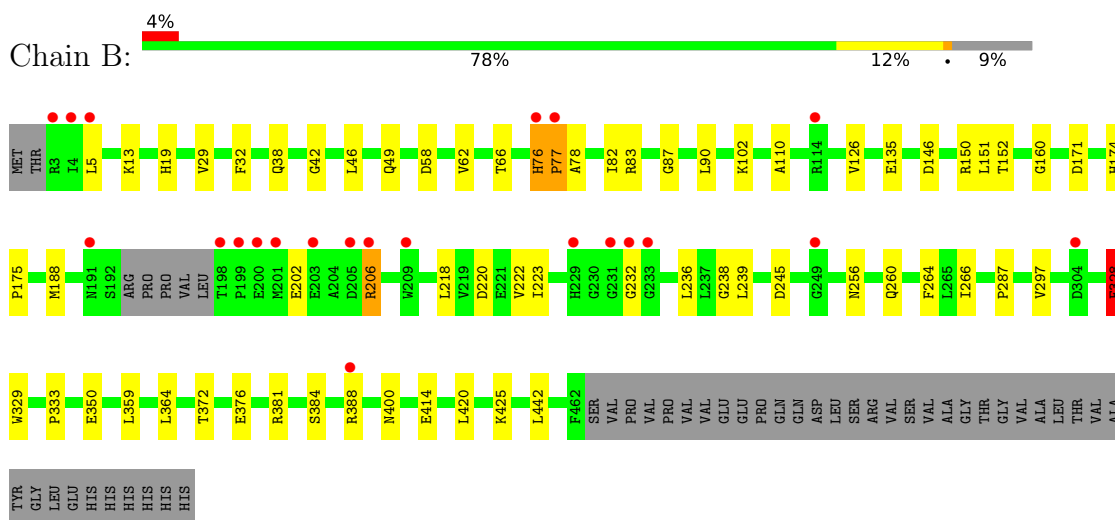
### 3 Residue-property plots

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: Bifunctional cytochrome P450/NADPH-P450 reductase

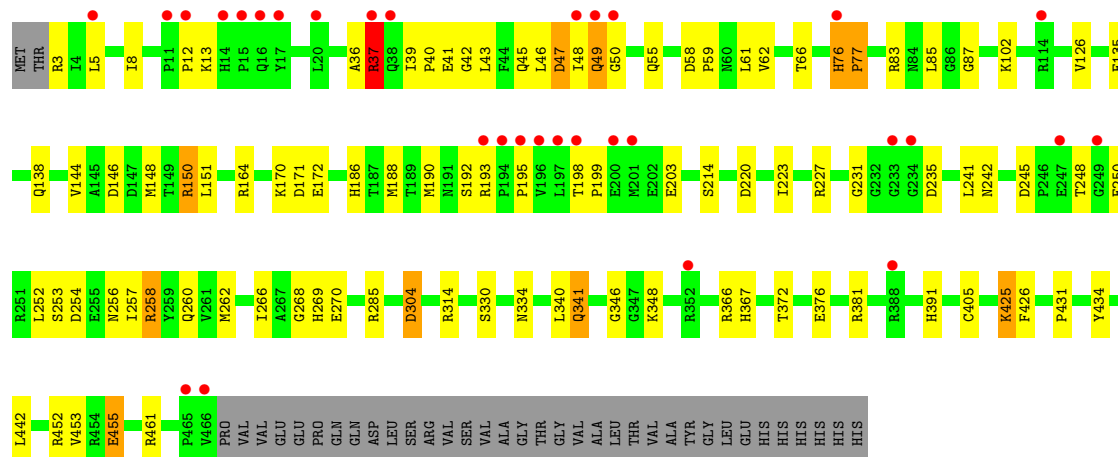


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	426.30Å 62.80Å 95.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50 29.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.00-2.50) 89.2 (29.18-2.50)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, $R_{free}$	0.200 , 0.246 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	1929 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, SO4

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	0.64	7/3820 (0.2%)	1.03	30/5185 (0.6%)
1	B	0.51	0/3756	0.70	4/5095 (0.1%)
1	C	0.53	1/3704 (0.0%)	0.96	19/5028 (0.4%)
1	D	0.59	4/3827 (0.1%)	0.87	18/5197 (0.3%)
All	All	0.57	12/15107 (0.1%)	0.90	71/20505 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	14

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	HIS	C-N	10.98	1.55	1.34
1	A	172	GLU	CD-OE2	8.31	1.34	1.25
1	D	203	GLU	CG-CD	7.86	1.63	1.51
1	A	221	GLU	CD-OE2	7.34	1.33	1.25
1	C	425	LYS	CB-CG	-7.07	1.33	1.52
1	A	172	GLU	CD-OE1	-6.96	1.18	1.25
1	A	221	GLU	CD-OE1	5.80	1.32	1.25
1	A	414	GLU	CD-OE2	5.78	1.32	1.25
1	D	455	GLU	CD-OE2	5.69	1.31	1.25
1	A	221	GLU	CG-CD	5.59	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	455	GLU	CB-CG	-5.05	1.42	1.52
1	D	341	GLN	CD-NE2	5.03	1.45	1.32

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLU	OE1-CD-OE2	-19.88	99.44	123.30
1	C	454	ARG	NE-CZ-NH1	-19.11	110.75	120.30
1	C	227	ARG	NE-CZ-NH2	18.00	129.30	120.30
1	C	454	ARG	NE-CZ-NH2	17.19	128.90	120.30
1	A	76	HIS	N-CA-C	-14.21	72.62	111.00
1	A	76	HIS	N-CA-CB	13.16	134.29	110.60
1	D	37	ARG	NE-CZ-NH1	-12.84	113.88	120.30
1	C	227	ARG	CA-CB-CG	-12.69	85.47	113.40
1	C	227	ARG	CB-CG-CD	12.64	144.46	111.60
1	A	221	GLU	CA-CB-CG	12.17	140.18	113.40
1	A	172	GLU	CG-CD-OE1	12.03	142.35	118.30
1	A	76	HIS	CB-CA-C	-11.34	87.72	110.40
1	D	304	ASP	CB-CG-OD1	-11.08	108.33	118.30
1	A	51	ARG	CB-CG-CD	-10.88	83.32	111.60
1	A	3	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	D	304	ASP	CB-CG-OD2	10.06	127.35	118.30
1	C	227	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	C	445	LYS	CD-CE-NZ	-9.83	89.08	111.70
1	A	414	GLU	OE1-CD-OE2	-9.74	111.62	123.30
1	C	4	ILE	CG1-CB-CG2	-9.68	90.11	111.40
1	A	224	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	D	37	ARG	NE-CZ-NH2	9.17	124.89	120.30
1	A	225	GLU	CG-CD-OE2	-8.94	100.43	118.30
1	C	381	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	C	454	ARG	CD-NE-CZ	8.52	135.53	123.60
1	D	36	ALA	C-N-CA	-8.51	100.44	121.70
1	B	206	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	229	HIS	CB-CA-C	-8.22	93.97	110.40
1	A	172	GLU	CG-CD-OE2	-7.94	102.42	118.30
1	C	381	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	B	206	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	D	47	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	A	221	GLU	N-CA-CB	-7.25	97.55	110.60
1	A	225	GLU	CB-CA-C	6.89	124.18	110.40
1	A	85	LEU	CA-CB-CG	6.86	131.07	115.30
1	C	454	ARG	CB-CA-C	6.71	123.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	430	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	258	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	D	268	GLY	C-N-CA	-6.54	105.34	121.70
1	D	85	LEU	CA-CB-CG	6.45	130.13	115.30
1	C	425	LYS	CA-CB-CG	6.34	127.35	113.40
1	A	225	GLU	N-CA-CB	-6.32	99.23	110.60
1	A	224	ARG	CD-NE-CZ	6.30	132.42	123.60
1	A	225	GLU	CA-CB-CG	6.28	127.20	113.40
1	D	47	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	328	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	D	150	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	D	47	ASP	N-CA-C	-5.72	95.55	111.00
1	D	37	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	A	163	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	B	359	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	D	47	ASP	CB-CA-C	5.63	121.67	110.40
1	A	47	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	3	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	C	381	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	47	ASP	N-CA-CB	5.41	120.34	110.60
1	D	340	LEU	C-N-CA	5.31	134.98	121.70
1	C	227	ARG	CG-CD-NE	5.29	122.91	111.80
1	A	3	ARG	CG-CD-NE	-5.25	100.78	111.80
1	A	51	ARG	CA-CB-CG	5.24	124.94	113.40
1	C	268	GLY	C-N-CA	-5.21	108.69	121.70
1	D	47	ASP	N-CA-CB	-5.19	101.25	110.60
1	D	258	ARG	CA-CB-CG	5.17	124.78	113.40
1	A	224	ARG	CB-CG-CD	-5.16	98.17	111.60
1	D	461	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	225	GLU	C-N-CA	5.14	134.56	121.70
1	C	217	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	224	ARG	CA-CB-CG	5.05	124.50	113.40
1	C	237	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	A	229	HIS	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	TYR	Sidechain
1	A	172	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	A	224	ARG	Peptide
1	A	225	GLU	Sidechain,Peptide
1	A	228	GLY	Peptide
1	A	414	GLU	Sidechain
1	A	75	VAL	Peptide
1	A	76	HIS	Sidechain
1	B	328	PHE	Sidechain
1	C	228	GLY	Peptide
1	C	454	ARG	Sidechain
1	D	341	GLN	Sidechain
1	D	46	LEU	Peptide

## 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	3725	0	3680	61	0
1	B	3664	0	3610	39	0
1	C	3611	0	3573	70	0
1	D	3731	0	3688	62	0
2	A	43	0	30	6	0
2	B	43	0	30	1	0
2	C	43	0	30	5	0
2	D	43	0	30	4	0
3	A	10	0	0	0	0
3	D	5	0	0	0	0
4	B	6	0	4	0	0
5	A	79	0	0	4	0
5	B	69	0	0	0	0
5	C	55	0	0	1	0
5	D	65	0	0	3	0
All	All	15192	0	14675	237	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 8.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:NH2	1:C:254:ASP:OD1	1.90	1.04
1:A:224:ARG:HG2	1:A:225:GLU:HB2	1.50	0.91
1:D:227:ARG:NH1	1:D:254:ASP:OD1	2.07	0.88
1:A:76:HIS:HB2	1:A:77:PRO:HD3	1.57	0.86
1:A:55:GLN:HE22	1:A:334:ASN:HD21	1.23	0.85
1:A:76:HIS:HB2	1:A:77:PRO:CD	2.08	0.82
1:D:76:HIS:HB3	1:D:77:PRO:HD3	1.63	0.80
1:D:42:GLY:HA3	1:D:58:ASP:HB2	1.65	0.78
1:C:55:GLN:HE22	1:C:334:ASN:HD21	1.31	0.77
1:A:372:THR:O	1:A:381:ARG:NH2	2.18	0.77
1:B:150:ARG:NH2	1:B:171:ASP:O	2.20	0.74
1:D:146:ASP:OD2	1:D:150:ARG:NH1	2.21	0.74
1:C:231:GLY:HA3	1:C:238:GLY:HA2	1.69	0.73
1:B:135:GLU:OE1	1:B:425:LYS:NZ	2.21	0.72
1:C:135:GLU:OE2	1:C:425:LYS:HE3	1.91	0.71
1:C:156:ILE:HG23	1:C:265:LEU:HD22	1.74	0.70
1:C:227:ARG:HE	1:C:241:LEU:HD22	1.56	0.70
1:D:372:THR:O	1:D:381:ARG:NH2	2.26	0.69
1:C:226:ARG:NH2	1:C:235:ASP:OD2	2.25	0.68
1:D:102:LYS:HE2	1:D:252:LEU:HD23	1.73	0.68
1:D:43:LEU:HD23	1:D:61:LEU:HD13	1.74	0.68
1:A:146:ASP:OD2	1:A:150:ARG:NH1	2.26	0.68
1:A:290:LEU:HD23	1:B:287:PRO:HB2	1.73	0.68
1:B:372:THR:O	1:B:381:ARG:NH2	2.28	0.67
1:D:262:MET:O	1:D:266:ILE:HG12	1.94	0.67
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.77	0.67
1:C:372:THR:O	1:C:381:ARG:NH2	2.28	0.66
1:C:227:ARG:NE	1:C:241:LEU:HD22	2.11	0.65
1:A:42:GLY:HA3	1:A:58:ASP:HB2	1.79	0.65
1:D:245:ASP:OD2	1:D:248:THR:HG22	1.96	0.64
1:D:431:PRO:HG3	1:D:452:ARG:HG3	1.78	0.64
1:B:202:GLU:O	1:B:206:ARG:HG3	1.98	0.63
1:A:297:VAL:HG22	1:A:420:LEU:HD12	1.80	0.63
1:A:364:LEU:HD11	1:A:394:ALA:HA	1.80	0.62
1:D:8:ILE:HG12	1:D:43:LEU:HD11	1.80	0.62
1:D:220:ASP:OD1	1:D:258:ARG:HG3	1.98	0.62
1:D:76:HIS:CB	1:D:77:PRO:HD3	2.29	0.62
1:C:244:THR:O	1:C:246:PRO:HD3	1.99	0.61
2:A:601:HEM:HMC1	2:A:601:HEM:HBC2	1.81	0.61
1:A:74:ARG:HB3	1:A:76:HIS:CD2	2.36	0.61
1:C:340:LEU:O	1:C:353:LYS:HG3	2.01	0.60
1:A:66:THR:HG23	1:A:400:ASN:OD1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:O	1:A:225:GLU:HB3	2.00	0.60
1:A:76:HIS:CB	1:A:77:PRO:HD3	2.26	0.60
1:A:221:GLU:O	1:A:225:GLU:CB	2.49	0.60
1:A:76:HIS:H	1:A:77:PRO:CD	2.12	0.60
1:C:106:ILE:HD12	1:C:252:LEU:HG	1.84	0.59
1:A:136:ARG:NH1	5:A:705:HOH:O	2.35	0.59
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.85	0.59
1:C:454:ARG:HH11	1:D:376:GLU:HG2	1.67	0.58
1:B:110:ALA:HB2	1:B:239:LEU:HD13	1.85	0.58
1:C:135:GLU:OE2	1:C:425:LYS:CE	2.51	0.58
1:C:225:GLU:O	1:C:229:HIS:ND1	2.36	0.58
1:D:48:ILE:O	1:D:50:GLY:N	2.37	0.58
1:D:55:GLN:HE22	1:D:334:ASN:HD21	1.49	0.58
1:D:269:HIS:CE1	1:D:270:GLU:HG3	2.37	0.58
1:B:146:ASP:OD2	1:B:150:ARG:NH1	2.36	0.57
2:C:601:HEM:HBB2	2:C:601:HEM:HMB2	1.86	0.57
1:C:136:ARG:NH1	5:C:702:HOH:O	2.36	0.57
1:A:37:ARG:NH1	5:A:706:HOH:O	2.35	0.57
1:D:186:HIS:O	1:D:190:MET:HG3	2.05	0.57
1:C:82:ILE:HD11	1:C:266:ILE:HG21	1.85	0.57
1:D:62:VAL:O	1:D:66:THR:OG1	2.16	0.57
1:D:198:THR:HB	1:D:199:PRO:HD2	1.85	0.57
1:D:170:LYS:HE2	1:D:172:GLU:HB2	1.87	0.57
1:C:174:HIS:O	1:C:178:GLN:HG3	2.05	0.57
1:C:20:LEU:HD11	1:C:49:GLN:HG3	1.87	0.56
1:A:152:THR:HG22	1:A:414:GLU:OE1	2.05	0.56
1:A:232:GLY:HA2	1:A:238:GLY:HA3	1.87	0.56
1:A:66:THR:HG21	5:A:768:HOH:O	2.04	0.56
1:B:174:HIS:ND1	1:B:175:PRO:HD2	2.21	0.56
1:D:188:MET:HE3	1:D:442:LEU:HB2	1.88	0.56
1:A:190:MET:HG2	1:A:193:ARG:NH2	2.21	0.56
1:A:198:THR:HB	1:A:199:PRO:HD2	1.88	0.55
1:C:157:SER:HB3	1:C:165:PHE:HE2	1.72	0.55
1:D:126:VAL:HG12	1:D:151:LEU:HD12	1.87	0.55
1:C:217:GLU:O	1:C:221:GLU:HG3	2.05	0.55
1:D:135:GLU:OE2	1:D:425:LYS:NZ	2.39	0.55
1:D:253:SER:O	1:D:257:ILE:HG13	2.07	0.55
1:C:214:SER:O	1:C:217:GLU:HB3	2.08	0.54
1:C:297:VAL:HG22	1:C:420:LEU:HD12	1.90	0.54
1:D:188:MET:HE1	1:D:442:LEU:HD12	1.89	0.54
1:D:3:ARG:HH22	1:D:5:LEU:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:OD2	1:A:387:ARG:NH2	2.41	0.54
1:C:126:VAL:HG21	1:C:155:THR:HA	1.90	0.53
2:D:601:HEM:HBC2	2:D:601:HEM:HMC2	1.90	0.53
1:C:138:GLN:NE2	1:C:455:GLU:HG3	2.24	0.53
1:C:234:GLY:O	1:C:235:ASP:HB2	2.09	0.52
1:D:39:ILE:HG22	1:D:41:GLU:OE1	2.10	0.52
1:D:192:SER:O	1:D:193:ARG:HG2	2.10	0.52
1:A:271:THR:HB	2:A:601:HEM:C2C	2.46	0.51
1:B:102:LYS:HG2	1:B:245:ASP:OD2	2.10	0.51
1:B:297:VAL:HG22	1:B:420:LEU:HD12	1.92	0.51
1:C:188:MET:CE	1:C:442:LEU:HB2	2.41	0.50
1:C:73:LYS:HE3	1:C:79:TYR:CZ	2.47	0.50
1:B:218:LEU:O	1:B:222:VAL:HG23	2.12	0.50
1:D:256:ASN:O	1:D:260:GLN:HG2	2.10	0.50
1:C:244:THR:HG22	1:C:251:ARG:HG3	1.94	0.50
1:D:346:GLY:O	1:D:348:LYS:HG3	2.11	0.50
1:A:163:TYR:HD1	1:A:164:ARG:N	2.10	0.49
1:C:48:ILE:O	1:C:49:GLN:C	2.51	0.49
1:C:184:MET:SD	1:C:266:ILE:HD12	2.52	0.49
1:A:12:PRO:O	1:A:13:LYS:HB3	2.13	0.49
1:B:188:MET:HE3	1:B:442:LEU:HB2	1.95	0.49
1:B:42:GLY:HA3	1:B:58:ASP:HB2	1.93	0.49
1:B:328:PHE:HB3	1:B:329:TRP:CD1	2.46	0.49
1:C:262:MET:O	1:C:266:ILE:HG12	2.13	0.49
1:D:8:ILE:CG2	1:D:45:GLN:HG2	2.41	0.49
1:D:248:THR:HG23	1:D:250:GLU:CG	2.41	0.49
1:C:407:GLY:HA3	2:C:601:HEM:C2B	2.47	0.49
1:B:29:VAL:HG21	1:B:333:PRO:HB2	1.94	0.49
1:D:138:GLN:HE22	1:D:455:GLU:HG3	1.78	0.49
1:A:262:MET:O	1:A:266:ILE:HG12	2.12	0.48
1:C:215:MET:O	1:C:219:VAL:HG23	2.13	0.48
1:B:188:MET:CE	1:B:442:LEU:HB2	2.43	0.48
1:C:364:LEU:HD11	1:C:394:ALA:HA	1.95	0.48
1:D:405:CYS:HB2	2:D:601:HEM:NA	2.28	0.48
1:A:130:LEU:HD21	1:A:422:ILE:HD11	1.96	0.48
1:D:248:THR:HG23	1:D:250:GLU:HG2	1.96	0.47
1:D:41:GLU:OE1	1:D:41:GLU:N	2.46	0.47
1:A:76:HIS:CE1	1:A:338:THR:HG21	2.49	0.47
1:B:13:LYS:HD3	1:B:19:HIS:NE2	2.29	0.47
1:A:53:LEU:HD12	5:A:755:HOH:O	2.15	0.47
1:A:77:PRO:HD2	1:A:78:ALA:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:O	1:A:225:GLU:HB2	2.15	0.47
1:B:160:GLY:HA2	1:B:236:LEU:HB2	1.96	0.47
1:C:127:ALA:O	1:C:130:LEU:HB3	2.15	0.46
1:C:240:MET:HE2	1:C:257:ILE:HG23	1.97	0.46
1:D:12:PRO:O	1:D:13:LYS:HB2	2.15	0.46
1:D:76:HIS:HB3	1:D:77:PRO:CD	2.39	0.46
1:D:144:VAL:O	1:D:148:MET:HG2	2.15	0.46
1:B:256:ASN:O	1:B:260:GLN:HG2	2.15	0.46
1:D:37:ARG:HH11	1:D:37:ARG:HD2	1.48	0.46
1:A:227:ARG:CZ	1:A:241:LEU:HD22	2.45	0.46
1:C:156:ILE:CG2	1:C:265:LEU:HD22	2.45	0.46
1:B:384:SER:O	1:B:388:ARG:HG3	2.16	0.46
1:C:307:PRO:HG3	1:C:421:LEU:HD21	1.97	0.46
1:C:256:ASN:O	1:C:260:GLN:HG2	2.16	0.46
1:C:103:ALA:HB1	1:C:260:GLN:NE2	2.31	0.46
1:C:188:MET:HE3	1:C:442:LEU:HB2	1.96	0.46
1:A:188:MET:HE3	1:A:442:LEU:HB2	1.98	0.46
1:B:66:THR:HG23	1:B:400:ASN:OD1	2.16	0.46
1:B:76:HIS:O	1:B:77:PRO:C	2.55	0.46
1:C:102:LYS:HG3	1:C:245:ASP:OD1	2.16	0.46
1:A:335:TYR:CZ	1:A:399:GLY:HA2	2.51	0.45
1:A:340:LEU:O	1:A:353:LYS:HG3	2.16	0.45
1:B:126:VAL:HG12	1:B:151:LEU:HD12	1.98	0.45
1:C:228:GLY:C	1:C:229:HIS:CG	2.89	0.45
1:C:310:ASP:OD2	1:C:314:ARG:NH2	2.39	0.45
1:A:193:ARG:HB2	1:A:194:PRO:CD	2.46	0.45
1:A:326:LEU:HD22	2:A:601:HEM:HBC1	1.97	0.45
1:B:38:GLN:OE1	1:D:214:SER:HB3	2.16	0.45
1:D:8:ILE:HG22	1:D:45:GLN:HG2	1.98	0.45
1:C:42:GLY:HA3	1:C:58:ASP:HB2	1.99	0.45
1:C:106:ILE:CD1	1:C:252:LEU:HG	2.45	0.45
1:C:127:ALA:HB1	1:C:421:LEU:HD12	1.97	0.45
1:A:59:PRO:HD3	1:A:367:HIS:CD2	2.52	0.45
1:B:83:ARG:HG3	1:B:87:GLY:O	2.16	0.45
1:C:188:MET:HE1	1:C:442:LEU:HD13	1.98	0.45
1:D:188:MET:CE	1:D:442:LEU:HB2	2.47	0.45
1:D:366:ARG:NH2	5:D:714:HOH:O	2.49	0.45
1:A:76:HIS:N	1:A:77:PRO:CD	2.69	0.45
1:A:376:GLU:O	1:A:381:ARG:NH1	2.50	0.45
1:C:425:LYS:O	1:C:456:ARG:HG3	2.16	0.45
1:D:59:PRO:HB2	1:D:391:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HG12	1:A:151:LEU:HD12	1.99	0.45
1:A:188:MET:HE1	1:A:442:LEU:HD13	1.99	0.45
1:B:188:MET:HE1	1:B:442:LEU:HD13	1.99	0.45
1:D:83:ARG:HG3	1:D:87:GLY:O	2.16	0.45
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.99	0.44
1:D:164:ARG:HA	5:D:736:HOH:O	2.15	0.44
1:C:103:ALA:CB	1:C:260:GLN:NE2	2.80	0.44
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.44	0.44
1:C:226:ARG:HG2	1:C:231:GLY:HA2	1.99	0.44
1:A:287:PRO:HB3	1:B:287:PRO:HB3	1.99	0.44
1:A:244:THR:HG22	1:A:251:ARG:HG3	2.00	0.44
1:C:75:VAL:HG13	1:C:79:TYR:HB2	2.01	0.43
1:B:110:ALA:HB2	1:B:239:LEU:CD1	2.48	0.43
1:B:232:GLY:HA3	1:B:238:GLY:HA2	2.00	0.43
1:C:221:GLU:HG2	1:C:224:ARG:NH2	2.33	0.43
1:D:43:LEU:HD23	1:D:61:LEU:CD1	2.47	0.43
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.47	0.43
1:C:236:LEU:HD13	1:C:264:PHE:CE2	2.54	0.43
1:C:133:LYS:NZ	1:C:147:ASP:OD1	2.45	0.43
1:B:220:ASP:HA	1:B:223:ILE:HD12	2.01	0.43
1:A:193:ARG:HB2	1:A:194:PRO:HD2	2.00	0.43
1:C:154:ASP:OD1	1:C:167:SER:OG	2.29	0.43
1:D:150:ARG:NH2	1:D:171:ASP:O	2.50	0.43
1:B:376:GLU:O	1:B:381:ARG:NH1	2.51	0.43
1:C:76:HIS:O	1:C:77:PRO:C	2.57	0.43
1:D:3:ARG:NH2	1:D:5:LEU:HD12	2.34	0.43
1:C:231:GLY:HA3	1:C:238:GLY:CA	2.43	0.42
1:C:84:ASN:HD22	1:C:190:MET:HE1	1.84	0.42
1:C:327:ARG:NH2	1:C:381:ARG:NH1	2.67	0.42
1:A:221:GLU:HA	1:A:224:ARG:HE	1.85	0.42
2:C:601:HEM:HBC2	2:C:601:HEM:CMC	2.49	0.42
1:A:232:GLY:HA2	1:A:238:GLY:CA	2.48	0.42
1:A:277:ALA:HB1	1:A:446:PRO:HG2	2.02	0.42
1:C:315:LEU:HB3	1:C:319:PRO:HD3	2.02	0.42
1:D:37:ARG:NH2	1:D:367:HIS:HA	2.34	0.42
1:D:348:LYS:HB3	1:D:348:LYS:HE2	1.80	0.42
1:D:138:GLN:NE2	1:D:455:GLU:HG3	2.35	0.42
1:D:285:ARG:NH2	1:D:434:TYR:O	2.50	0.42
1:A:221:GLU:CA	1:A:224:ARG:HH21	2.32	0.42
1:D:223:ILE:HG23	1:D:241:LEU:HD21	2.02	0.42
1:D:426:PHE:HB3	1:D:453:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HD13	1:B:264:PHE:CE2	2.55	0.41
2:B:602:HEM:HBB2	2:B:602:HEM:HMB2	2.02	0.41
1:C:157:SER:CB	1:C:165:PHE:HE2	2.33	0.41
1:A:203:GLU:HG2	1:A:206:ARG:HH12	1.86	0.41
1:A:80:THR:HG21	1:C:16:GLN:HE22	1.85	0.41
1:A:224:ARG:CG	1:A:225:GLU:HB2	2.36	0.41
1:C:227:ARG:HE	1:C:241:LEU:CD2	2.30	0.41
1:C:367:HIS:HA	1:C:368:PRO:HD3	1.97	0.41
1:A:110:ALA:HB2	1:A:239:LEU:HD13	2.03	0.41
1:B:62:VAL:HG21	1:B:364:LEU:HD13	2.02	0.41
1:C:328:PHE:HB3	1:C:329:TRP:CD1	2.55	0.41
1:D:231:GLY:O	1:D:242:ASN:ND2	2.53	0.41
1:B:152:THR:HA	1:B:414:GLU:OE2	2.19	0.41
1:A:150:ARG:NH2	1:A:171:ASP:O	2.54	0.41
1:B:32:PHE:CE1	1:B:46:LEU:HD11	2.55	0.41
1:C:42:GLY:HA2	1:C:57:TYR:CE1	2.56	0.41
1:D:48:ILE:O	1:D:49:GLN:C	2.59	0.41
1:D:227:ARG:CZ	1:D:241:LEU:HD22	2.51	0.41
1:A:221:GLU:HA	1:A:224:ARG:HH21	1.86	0.41
1:A:284:LEU:HD13	1:A:430:ASP:HB2	2.02	0.41
1:B:82:ILE:HD11	1:B:266:ILE:HG21	2.03	0.41
1:C:10:SER:HA	1:C:11:PRO:HD3	1.90	0.41
1:A:428:LEU:O	1:B:287:PRO:HD2	2.21	0.40
1:D:330:SER:HB3	5:D:724:HOH:O	2.20	0.40
1:D:314:ARG:H	1:D:314:ARG:HG2	1.76	0.40
1:B:5:LEU:HD13	1:B:350:GLU:HB2	2.03	0.40
1:B:90:LEU:HA	1:B:90:LEU:HD23	1.82	0.40
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.51	0.40
1:A:156:ILE:HD12	1:A:156:ILE:HA	1.85	0.40
1:A:407:GLY:HA3	2:A:601:HEM:C2B	2.56	0.40
1:C:108:LEU:HD23	1:C:108:LEU:HA	1.95	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	461/501 (92%)	440 (95%)	17 (4%)	4 (1%)	17	31
1	B	451/501 (90%)	432 (96%)	15 (3%)	4 (1%)	17	31
1	C	445/501 (89%)	421 (95%)	18 (4%)	6 (1%)	12	21
1	D	462/501 (92%)	435 (94%)	21 (4%)	6 (1%)	12	21
All	All	1819/2004 (91%)	1728 (95%)	71 (4%)	20 (1%)	14	26

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	B	76	HIS
1	B	77	PRO
1	C	77	PRO
1	C	235	ASP
1	D	49	GLN
1	D	76	HIS
1	A	49	GLN
1	A	77	PRO
1	B	49	GLN
1	C	78	ALA
1	C	49	GLN
1	C	227	ARG
1	C	229	HIS
1	D	77	PRO
1	D	195	PRO
1	D	235	ASP
1	B	78	ALA
1	D	40	PRO
1	A	193	ARG

### 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	391/423 (92%)	388 (99%)	3 (1%)	81	93
1	B	383/423 (90%)	383 (100%)	0	100	100
1	C	378/423 (89%)	376 (100%)	2 (0%)	88	96
1	D	392/423 (93%)	388 (99%)	4 (1%)	76	90
All	All	1544/1692 (91%)	1535 (99%)	9 (1%)	86	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	114	ARG
1	A	163	TYR
1	C	4	ILE
1	C	445	LYS
1	D	37	ARG
1	D	47	ASP
1	D	304	ASP
1	D	425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	B	76	HIS
1	B	356	GLN
1	C	16	GLN
1	C	84	ASN
1	C	334	ASN
1	D	186	HIS
1	D	334	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	601	1	41,50,50	1.41	6 (14%)	45,82,82	1.67	12 (26%)
3	SO4	D	602	-	4,4,4	0.31	0	6,6,6	0.24	0
2	HEM	B	602	1	41,50,50	1.42	4 (9%)	45,82,82	1.57	10 (22%)
2	HEM	D	601	1	41,50,50	1.55	5 (12%)	45,82,82	1.81	15 (33%)
3	SO4	A	602	-	4,4,4	0.32	0	6,6,6	0.13	0
2	HEM	C	601	1	41,50,50	1.51	8 (19%)	45,82,82	1.71	11 (24%)
3	SO4	A	603	-	4,4,4	0.41	0	6,6,6	0.25	0
4	SER	B	601	-	4,5,6	0.68	0	0,5,7	-	-

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	A	601	1	-	2/12/54/54	-
2	HEM	B	602	1	-	2/12/54/54	-
2	HEM	D	601	1	-	2/12/54/54	-
2	HEM	C	601	1	-	2/12/54/54	-
4	SER	B	601	-	-	0/2/4/6	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	C3C-C2C	-4.57	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-C2C	-3.79	1.35	1.40
2	D	601	HEM	C3C-CAC	3.53	1.55	1.47
2	C	601	HEM	C3C-C2C	-3.51	1.35	1.40
2	B	602	HEM	C3C-CAC	3.45	1.54	1.47
2	B	602	HEM	C3C-C2C	-3.41	1.35	1.40
2	C	601	HEM	CAB-C3B	2.93	1.55	1.47
2	A	601	HEM	CAB-C3B	2.75	1.54	1.47
2	B	602	HEM	CAB-C3B	2.69	1.54	1.47
2	A	601	HEM	FE-NB	2.65	2.10	1.96
2	C	601	HEM	FE-NB	2.55	2.09	1.96
2	D	601	HEM	CMB-C2B	2.52	1.56	1.50
2	C	601	HEM	CMB-C2B	2.51	1.56	1.50
2	C	601	HEM	CAA-C2A	2.49	1.55	1.52
2	C	601	HEM	C3C-CAC	2.42	1.52	1.47
2	C	601	HEM	C2C-C1C	2.37	1.47	1.42
2	C	601	HEM	CMC-C2C	2.32	1.57	1.51
2	A	601	HEM	C3C-CAC	2.31	1.52	1.47
2	A	601	HEM	CMD-C2D	2.29	1.55	1.50
2	D	601	HEM	CAB-C3B	2.26	1.53	1.47
2	D	601	HEM	CMC-C2C	2.26	1.56	1.51
2	A	601	HEM	C2C-C1C	2.13	1.47	1.42
2	B	602	HEM	FE-NB	2.01	2.06	1.96

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	C2C-C3C-C4C	4.10	109.76	106.90
2	B	602	HEM	CBA-CAA-C2A	-3.79	106.16	112.62
2	D	601	HEM	C4B-CHC-C1C	3.72	127.47	122.56
2	A	601	HEM	C2C-C3C-C4C	3.59	109.40	106.90
2	C	601	HEM	C4B-CHC-C1C	3.58	127.28	122.56
2	C	601	HEM	C1B-NB-C4B	3.43	108.62	105.07
2	A	601	HEM	CBD-CAD-C3D	-3.30	103.47	112.63
2	D	601	HEM	CAD-CBD-CGD	-3.29	106.53	113.60
2	D	601	HEM	C4D-ND-C1D	3.16	108.33	105.07
2	D	601	HEM	C4B-C3B-C2B	3.16	109.62	107.11
2	D	601	HEM	CBA-CAA-C2A	-3.14	107.26	112.62
2	A	601	HEM	CBA-CAA-C2A	-3.12	107.30	112.62
2	B	602	HEM	C4D-ND-C1D	3.09	108.26	105.07
2	C	601	HEM	CBA-CAA-C2A	-3.08	107.36	112.62
2	C	601	HEM	CBD-CAD-C3D	-3.04	104.18	112.63
2	C	601	HEM	C4C-CHD-C1D	3.04	126.57	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	HEM	C2C-C3C-C4C	2.93	108.95	106.90
2	B	602	HEM	C2C-C3C-C4C	2.86	108.89	106.90
2	D	601	HEM	O1D-CGD-CBD	-2.83	113.98	123.08
2	D	601	HEM	C1B-NB-C4B	2.82	107.99	105.07
2	A	601	HEM	O2A-CGA-CBA	2.81	123.07	114.03
2	A	601	HEM	C4B-CHC-C1C	2.80	126.26	122.56
2	B	602	HEM	C1B-NB-C4B	2.80	107.97	105.07
2	D	601	HEM	CHC-C4B-NB	2.80	127.47	124.43
2	D	601	HEM	C3D-C4D-ND	-2.79	107.06	110.17
2	A	601	HEM	C4D-ND-C1D	2.74	107.91	105.07
2	A	601	HEM	O1D-CGD-CBD	-2.58	114.78	123.08
2	C	601	HEM	C4D-ND-C1D	2.55	107.71	105.07
2	B	602	HEM	C4B-CHC-C1C	2.53	125.90	122.56
2	A	601	HEM	C1B-NB-C4B	2.53	107.68	105.07
2	D	601	HEM	C4C-CHD-C1D	2.52	125.89	122.56
2	A	601	HEM	C3D-C4D-ND	-2.48	107.41	110.17
2	B	602	HEM	C4C-CHD-C1D	2.41	125.73	122.56
2	C	601	HEM	C4B-C3B-C2B	2.30	108.94	107.11
2	C	601	HEM	CHC-C4B-NB	2.25	126.88	124.43
2	C	601	HEM	C4A-C3A-C2A	2.23	108.55	107.00
2	D	601	HEM	O2A-CGA-CBA	2.18	121.03	114.03
2	D	601	HEM	CHD-C1D-ND	2.18	126.80	124.43
2	C	601	HEM	CMC-C2C-C3C	2.15	128.70	124.68
2	D	601	HEM	CMC-C2C-C3C	2.15	128.69	124.68
2	B	602	HEM	CHC-C4B-NB	2.11	126.72	124.43
2	A	601	HEM	O1A-CGA-CBA	-2.10	116.33	123.08
2	B	602	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
2	B	602	HEM	C3D-C4D-ND	-2.07	107.86	110.17
2	A	601	HEM	CHC-C4B-NB	2.06	126.67	124.43
2	B	602	HEM	CMC-C2C-C3C	2.02	128.46	124.68
2	D	601	HEM	O1A-CGA-CBA	-2.01	116.61	123.08
2	A	601	HEM	CMC-C2C-C3C	2.01	128.44	124.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAD-CBD-CGD-O2D
2	B	602	HEM	CAD-CBD-CGD-O2D

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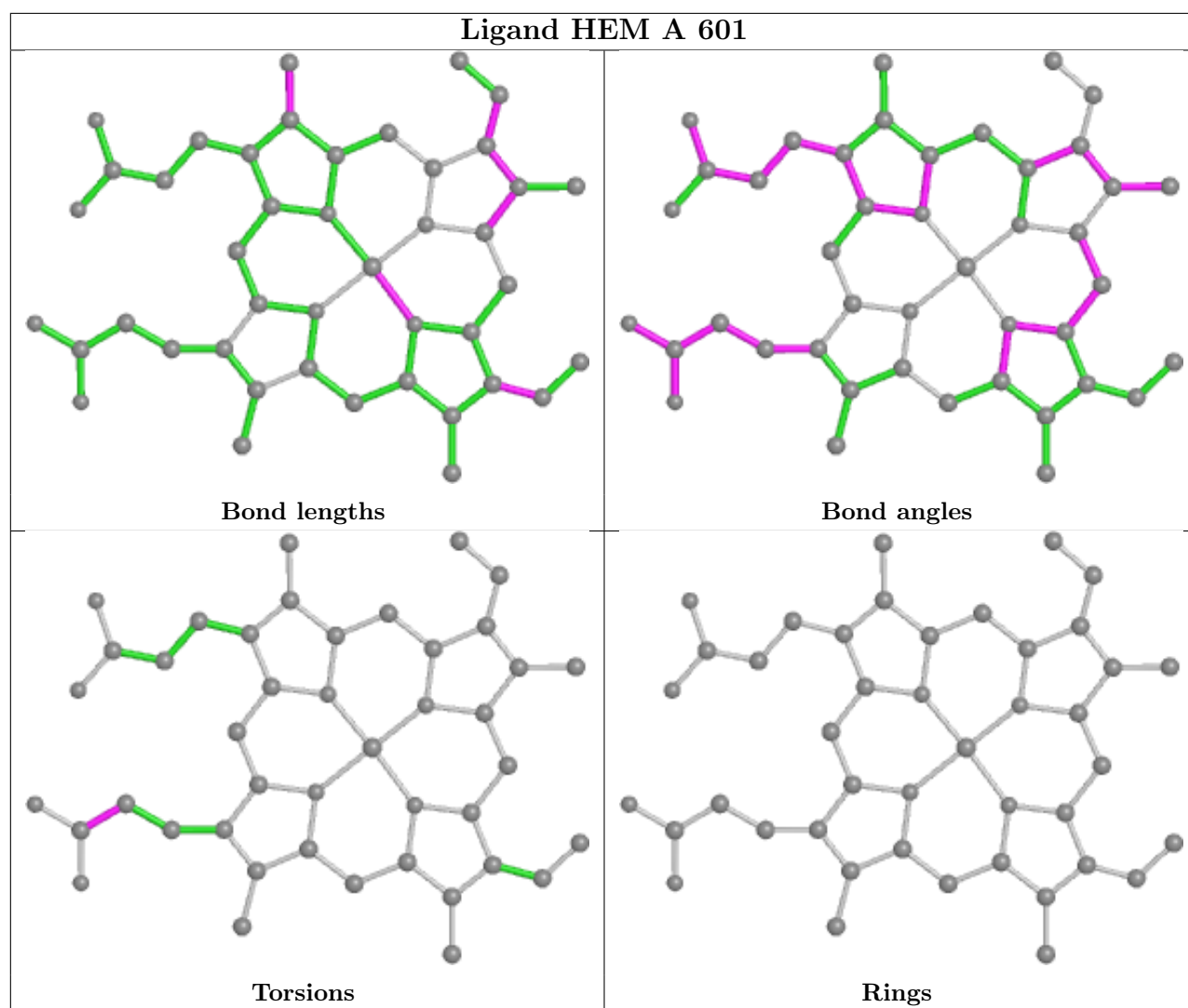
Mol	Chain	Res	Type	Atoms
2	B	602	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O2A

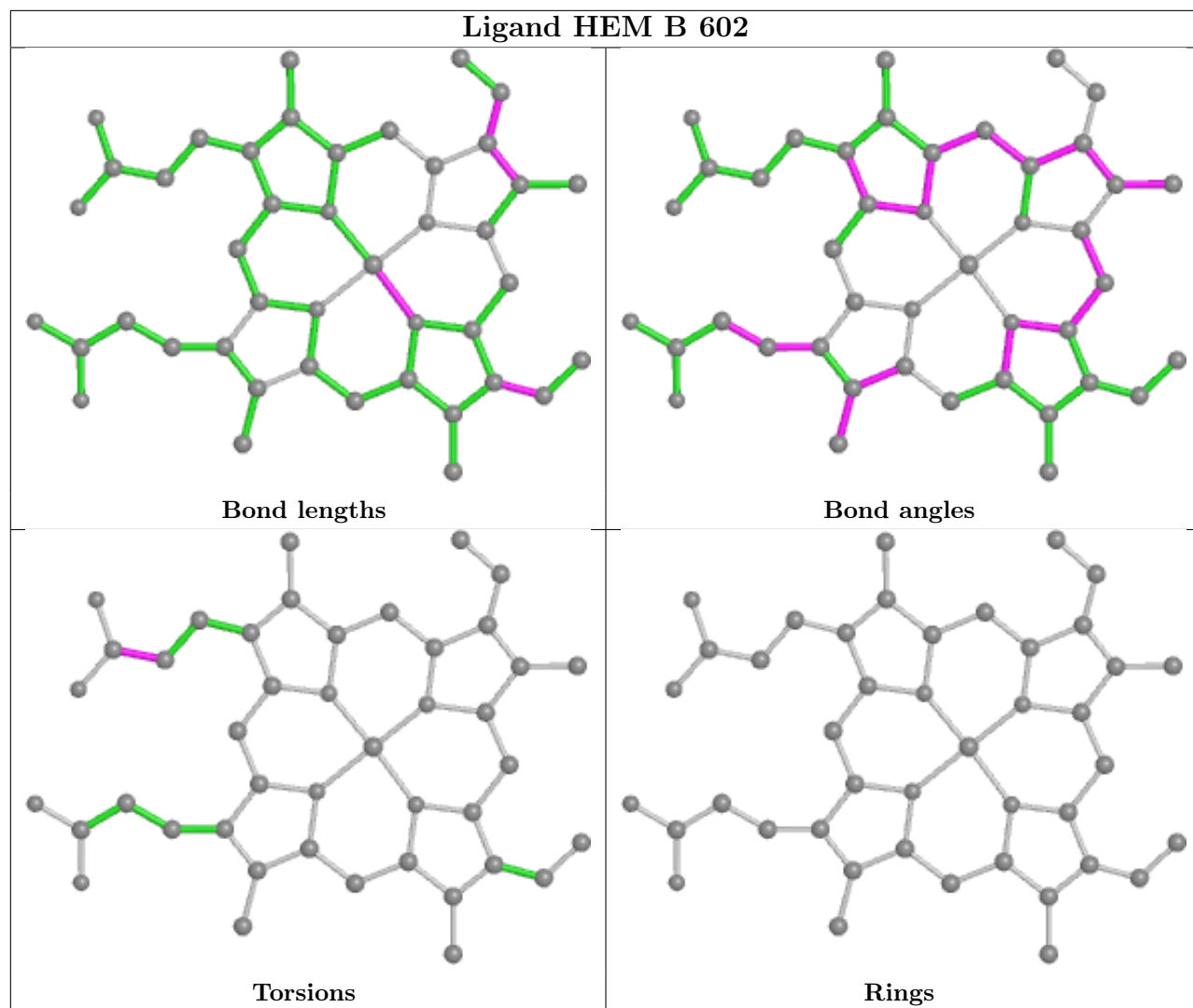
There are no ring outliers.

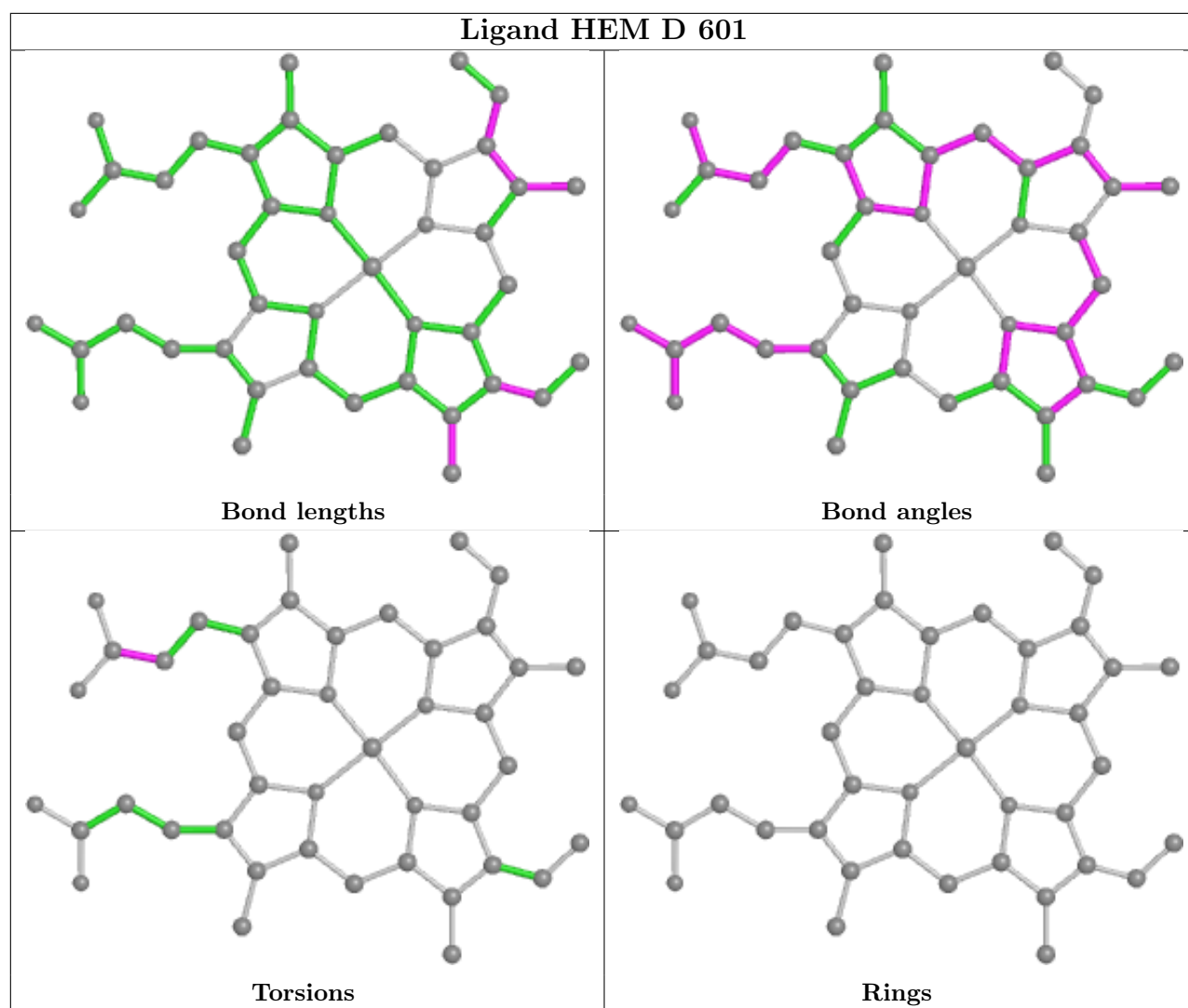
4 monomers are involved in 16 short contacts:

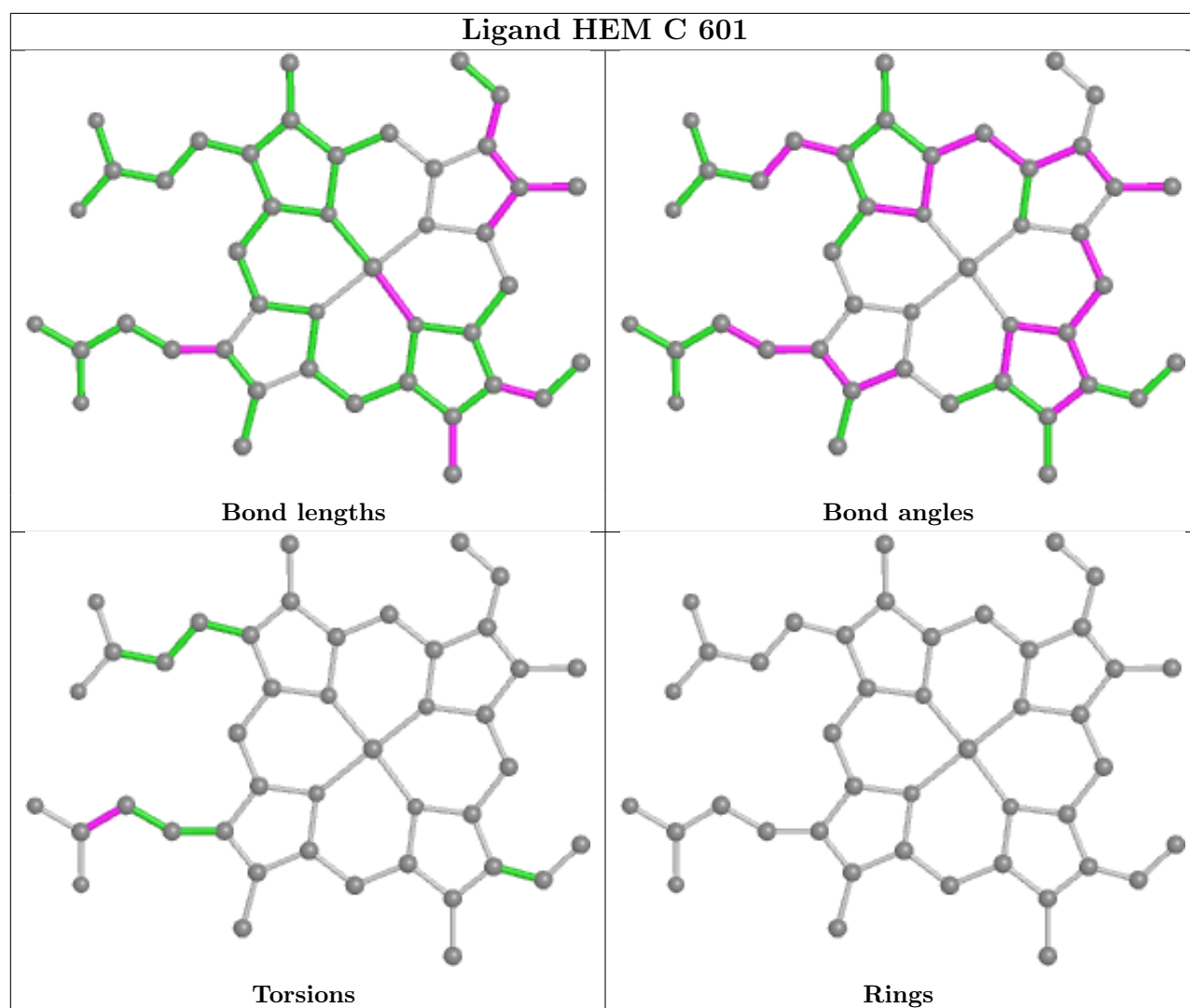
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	6	0
2	B	602	HEM	1	0
2	D	601	HEM	4	0
2	C	601	HEM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	462/501 (92%)	-0.02	24 (5%)	27	29	22, 33, 69, 126	0
1	B	455/501 (90%)	0.03	22 (4%)	30	32	22, 36, 67, 109	0
1	C	449/501 (89%)	0.22	36 (8%)	12	12	22, 39, 84, 118	0
1	D	464/501 (92%)	0.17	31 (6%)	17	18	20, 34, 77, 115	0
All	All	1830/2004 (91%)	0.10	113 (6%)	20	21	20, 35, 79, 126	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	PRO	8.9
1	B	76	HIS	7.7
1	C	229	HIS	7.1
1	A	231	GLY	7.0
1	B	229	HIS	6.6
1	C	234	GLY	6.5
1	D	17	TYR	6.2
1	C	233	GLY	6.1
1	A	196	VAL	6.1
1	C	232	GLY	6.0
1	A	194	PRO	5.9
1	C	467	PRO	5.8
1	A	464	VAL	5.8
1	D	196	VAL	5.8
1	C	230	GLY	5.8
1	D	49	GLN	5.6
1	D	16	GLN	5.3
1	C	3	ARG	5.2
1	D	200	GLU	5.1
1	D	466	VAL	4.9
1	D	198	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	229	HIS	4.7
1	A	76	HIS	4.7
1	B	77	PRO	4.6
1	C	209	TRP	4.6
1	B	231	GLY	4.5
1	D	15	PRO	4.5
1	C	208	TYR	4.4
1	C	182	ARG	4.3
1	C	223	ILE	4.3
1	C	466	VAL	4.3
1	D	193	ARG	4.3
1	B	199	PRO	4.2
1	B	4	ILE	4.2
1	A	4	ILE	4.2
1	C	388	ARG	4.1
1	B	232	GLY	4.0
1	A	197	LEU	4.0
1	D	194	PRO	4.0
1	C	77	PRO	3.9
1	A	49	GLN	3.9
1	A	198	THR	3.9
1	C	210	ALA	3.9
1	D	388	ARG	3.9
1	A	3	ARG	3.9
1	B	200	GLU	3.8
1	D	197	LEU	3.7
1	A	232	GLY	3.7
1	D	12	PRO	3.6
1	D	234	GLY	3.6
1	B	198	THR	3.6
1	C	207	ALA	3.6
1	C	244	THR	3.6
1	C	4	ILE	3.5
1	C	247	GLU	3.5
1	A	233	GLY	3.5
1	C	76	HIS	3.5
1	B	209	TRP	3.5
1	A	192	SER	3.5
1	D	50	GLY	3.5
1	B	114	ARG	3.4
1	D	20	LEU	3.4
1	B	206	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	203	GLU	3.4
1	A	230	GLY	3.4
1	D	233	GLY	3.4
1	C	249	GLY	3.4
1	D	201	MET	3.3
1	C	225	GLU	3.3
1	C	227	ARG	3.2
1	D	195	PRO	3.2
1	A	199	PRO	3.2
1	B	233	GLY	3.2
1	A	193	ARG	3.1
1	C	246	PRO	3.0
1	C	189	THR	2.9
1	A	50	GLY	2.9
1	D	465	PRO	2.8
1	C	186	HIS	2.8
1	A	463	SER	2.7
1	D	76	HIS	2.7
1	C	228	GLY	2.7
1	B	201	MET	2.7
1	C	185	HIS	2.6
1	B	249	GLY	2.6
1	A	114	ARG	2.6
1	D	14	HIS	2.6
1	A	201	MET	2.6
1	D	352	ARG	2.6
1	D	114	ARG	2.5
1	B	205	ASP	2.5
1	C	211	ASP	2.4
1	C	190	MET	2.4
1	C	231	GLY	2.4
1	B	5	LEU	2.4
1	D	11	PRO	2.3
1	B	3	ARG	2.3
1	C	175	PRO	2.3
1	B	191	ASN	2.3
1	B	388	ARG	2.3
1	C	174	HIS	2.3
1	D	48	ILE	2.3
1	A	191	ASN	2.2
1	D	247	GLU	2.2
1	D	249	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	5	LEU	2.1
1	C	188	MET	2.1
1	C	49	GLN	2.1
1	D	38	GLN	2.1
1	C	465	PRO	2.1
1	B	304	ASP	2.1
1	D	37	ARG	2.0
1	A	172	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

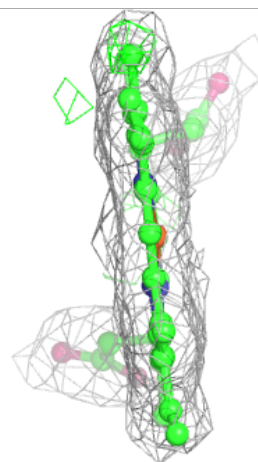
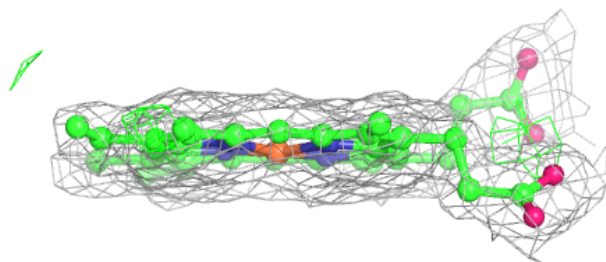
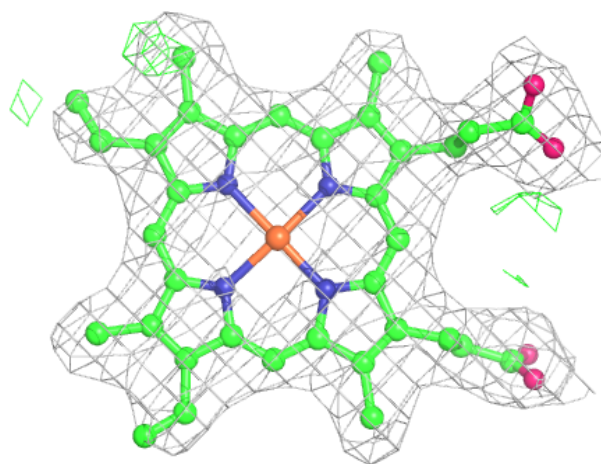
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SER	B	601	6/7	0.62	0.52	68,71,74,77	0
3	SO4	A	603	5/5	0.86	0.29	54,55,73,88	0
3	SO4	D	602	5/5	0.95	0.29	51,54,67,73	0
3	SO4	A	602	5/5	0.95	0.28	50,61,68,74	0
2	HEM	A	601	43/43	0.97	0.16	17,24,30,35	0
2	HEM	C	601	43/43	0.97	0.16	24,37,45,49	0
2	HEM	B	602	43/43	0.98	0.16	19,29,35,43	0
2	HEM	D	601	43/43	0.98	0.16	19,25,29,33	0

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

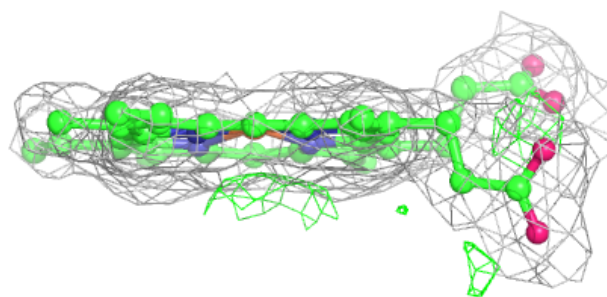
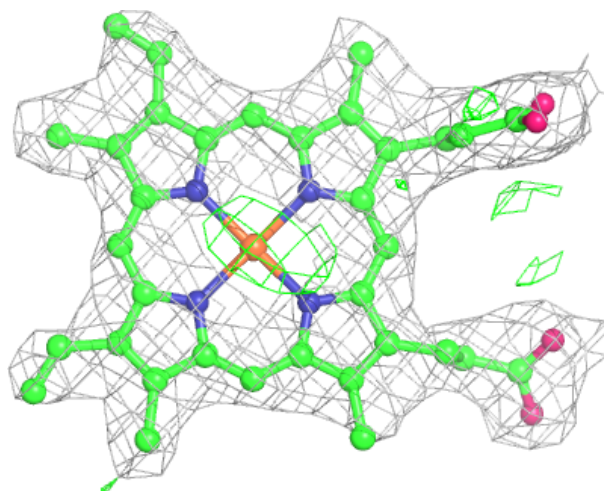
**Electron density around HEM A 601:**

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



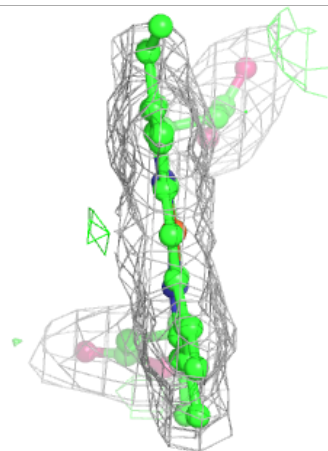
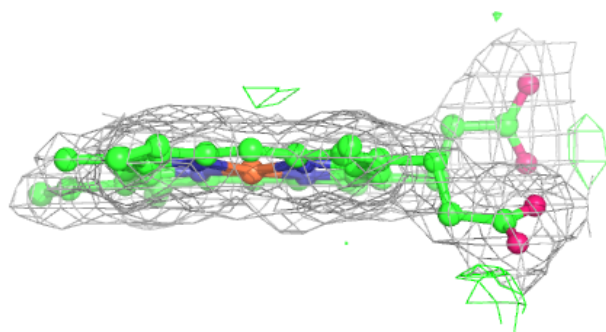
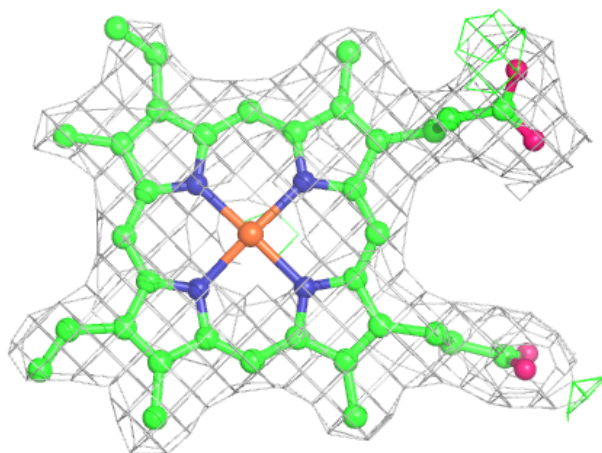
**Electron density around HEM C 601:**

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



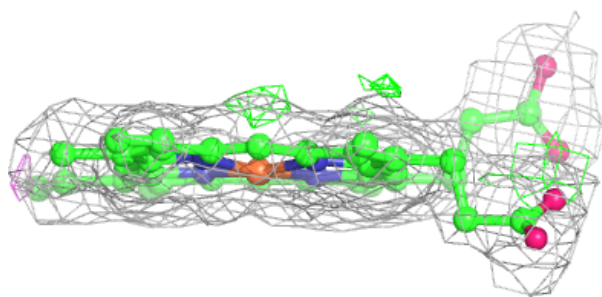
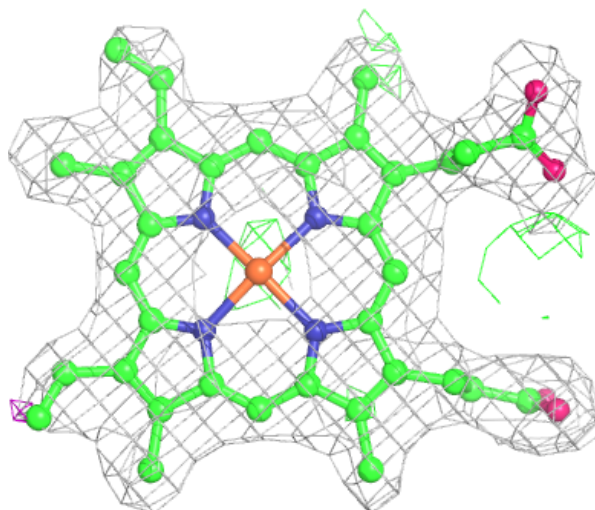
**Electron density around HEM B 602:**

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



**Electron density around HEM 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.