



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:02 am BST

PDB ID : 6O5Y
Title : Structure of Human Cytochrome P450 1A1 with 5-amino-N-(5-((4R,5R)-4-amino-5-fluoroazepan-1-yl)-1-methyl-1H-pyrazol-4-yl)-2-(2,6-difluorophenyl)thiazole-4-carboxamide)
Authors : Bart, A.G.; Scott, E.E.
Deposited on : 2019-03-04
Resolution : 3.17 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 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 : 2.11
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) : 2.11

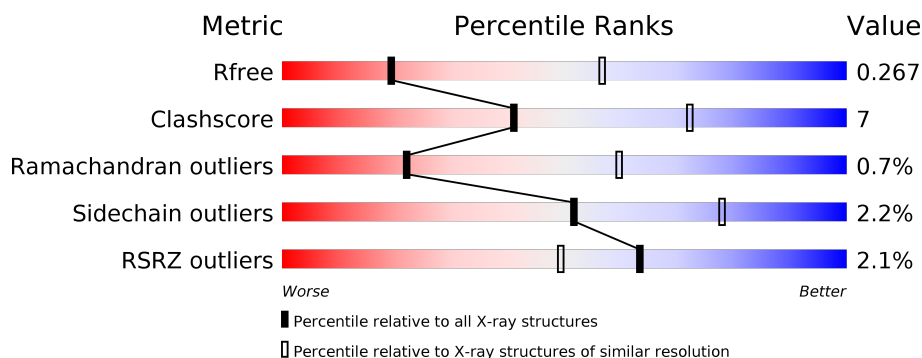
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 on 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	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 75%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 18% • 5% </div> </div>
1	B	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 82%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 13% • </div> </div>
1	C	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 15%, green 80%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 80% 15% • 5% </div> </div>
1	D	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 19%, green 73%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 73% 19% • 7% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30187 atoms, of which 15051 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 1A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	464	Total	C	H	N	O	S	0	0	0
			7441	2387	3720	647	666	21			
1	B	470	Total	C	H	N	O	S	0	0	0
			7552	2421	3776	657	678	20			
1	C	468	Total	C	H	N	O	S	0	0	0
			7488	2400	3743	651	673	21			
1	D	458	Total	C	H	N	O	S	0	0	0
			7346	2359	3670	639	658	20			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	initiating methionine	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

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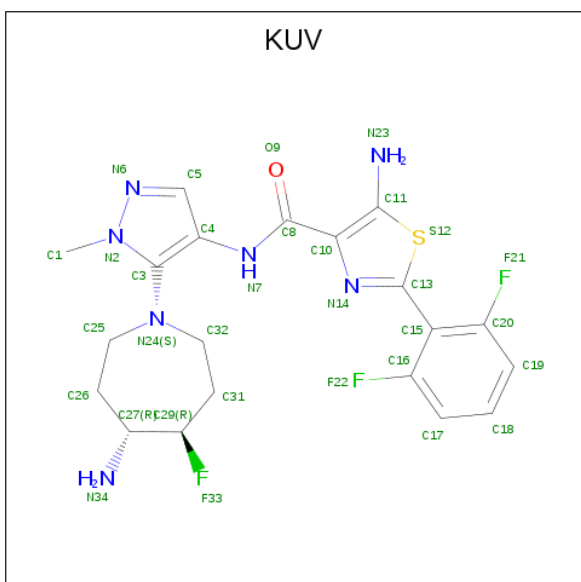
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	initiating methionine	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	initiating methionine	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

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



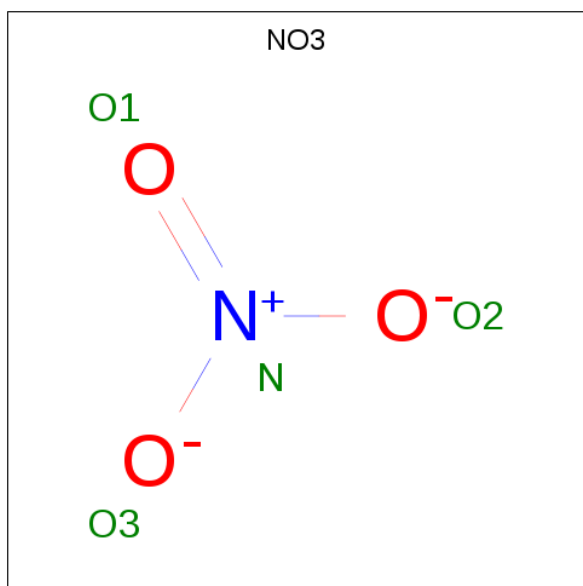
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is 5-amino-N-{5-[(4R,5R)-4-amino-5-fluoroazepan-1-yl]-1-methyl-1H-pyrazol-4-yl}-2-(2,6-difluorophenyl)-1,3-thiazole-4-carboxamide (three-letter code: KUV) (formula: $C_{20}H_{22}F_3N_7OS$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	S	0	0
			54	20	3	22	7	1	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		

These plots are drawn for all protein, RNA and DNA 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.

[illegible]

Chain B:

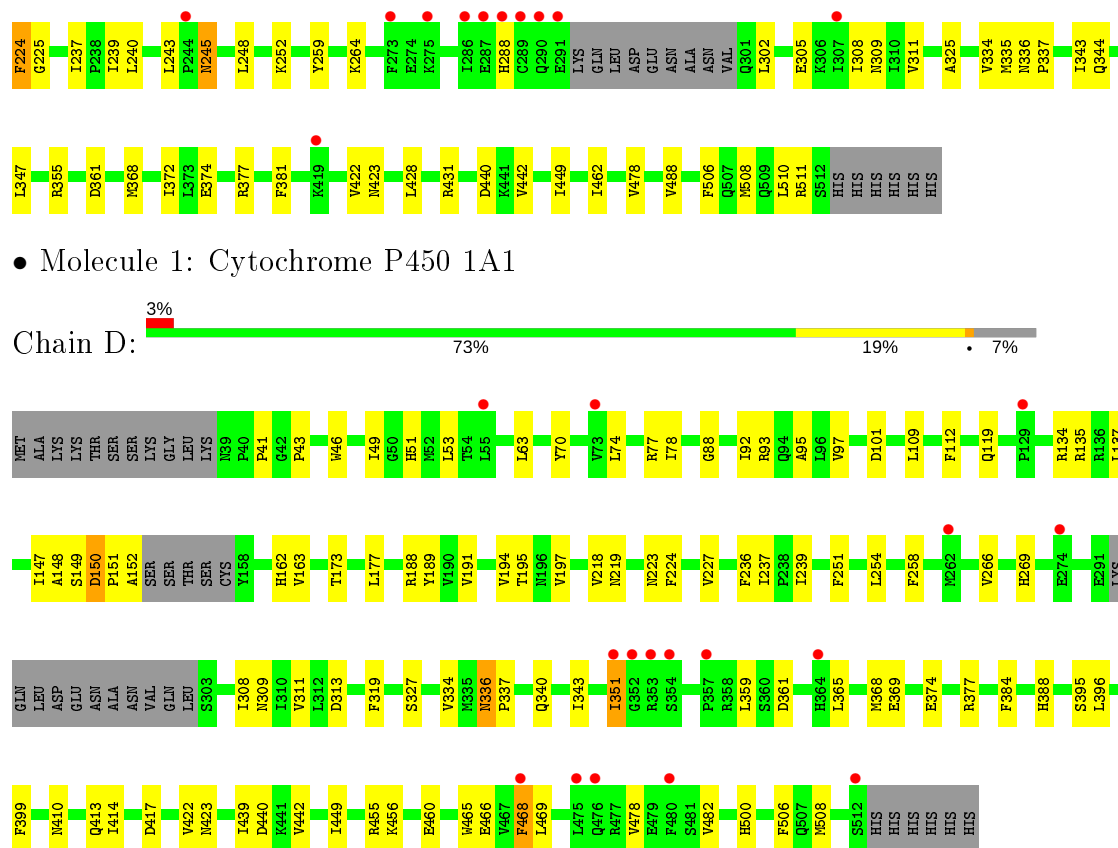
Residue	Color
MET	Red
ALA	Grey
LYS	Green
LYS	Green
THR	Yellow
THR	Yellow
SER	Grey
SER	Grey
LYS	Green
LYS	Green
GLY	Green
L37	Green
L49	Yellow
L53	Yellow
L63	Yellow
D72	Yellow
V73	Green
L74	Yellow
V85	Yellow
T91	Yellow
P151	Green
ALA	Grey
SER	Grey
SER	Grey
THR	Yellow
SER	Grey
SER	Grey
CYS	Blue
Y158	Yellow
S164	Yellow
V169	Yellow
L170	Green
I171	Yellow
H183	Yellow
P186	Yellow
Y187	Yellow
V190	Yellow
V191	Yellow
V194	Yellow
T195	Yellow
R206	Yellow
H211	Yellow
Q212	Green
E213	Yellow
L214	Yellow
L217	Green
L440	Yellow
R455	Green
K456	Yellow
E460	Yellow
T461	Green
I462	Yellow
A463	Yellow
R464	Yellow
W465	Green
E466	Yellow
L475	Yellow
Q476	Green
R477	Yellow
V478	Yellow
L484	Yellow
G485	Yellow
Y489	Yellow
G495	Yellow
F506	Yellow
Q507	Green
M508</	

Chain C:

3% 80% 15% 5%

• 5%

MET ALA LYS THR SER LYS G36 D72 V73 V74 L26 T91 I92 L114 Q119 V130 W131 R135 L142 S149 D150 P151 A152 S153 S154 T155 Y158 L159 V163 Q175 V192 Y207 D208 E209 N210 E211 Q212 E213 L214 L215 N221 N222 N223



● Molecule 1: Cytochrome P450 1A1

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.15Å 195.90Å 236.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.17 49.32 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.32-3.17) 85.9 (49.32-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14 _3260)	Depositor
R, R_{free}	0.239 , 0.267 0.240 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	30187	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: KUV, HEM, NO3

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	0.29	0/3814	0.47	0/5165
1	B	0.29	0/3870	0.48	0/5243
1	C	0.27	0/3839	0.45	0/5201
1	D	0.28	0/3769	0.45	0/5106
All	All	0.28	0/15292	0.46	0/20715

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3721	3720	3718	54	0
1	B	3776	3776	3773	37	0
1	C	3745	3743	3741	40	0
1	D	3676	3670	3667	61	0
2	A	43	30	30	9	0
2	B	43	30	30	4	0
2	C	43	30	30	6	0
2	D	43	30	30	6	0
3	A	32	22	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
All	All	15136	15051	15019	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (213) 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:119:GLN:O	1:C:309:ASN:ND2	2.06	0.89
1:D:351:ILE:HD11	1:D:365:LEU:HD11	1.65	0.77
1:A:359:LEU:HD21	1:A:465:TRP:CE3	2.19	0.76
1:B:478:VAL:HG13	1:B:508:MET:HG3	1.73	0.71
1:C:207:TYR:HB2	1:C:214:LEU:HD22	1.72	0.71
1:D:369:GLU:HB3	1:D:439:ILE:HD11	1.75	0.69
1:D:119:GLN:O	1:D:309:ASN:ND2	2.26	0.68
1:A:334:VAL:HG21	1:A:506:PHE:CE2	2.29	0.68
1:D:440:ASP:OD1	1:D:442:VAL:HG12	1.95	0.67
1:D:237:ILE:HG22	1:D:239:ILE:HG22	1.77	0.66
1:B:347:LEU:HD23	1:B:365:LEU:HD21	1.77	0.66
1:A:215:LEU:O	1:A:220:LEU:N	2.28	0.65
1:A:476:GLN:HG2	1:A:477:ARG:HG2	1.79	0.65
1:A:478:VAL:HG13	1:A:508:MET:HG3	1.80	0.64
1:B:169:VAL:HG11	1:B:206:ARG:HH21	1.63	0.63
1:A:237:ILE:HB	1:A:240:LEU:HD12	1.81	0.63
1:A:169:VAL:HG21	1:A:206:ARG:HH12	1.63	0.63
1:A:484:LEU:HD23	1:A:485:GLY:N	2.14	0.63
1:C:130:VAL:HG13	1:C:302:LEU:CD2	2.28	0.63
2:C:601:HEM:HH A	2:C:601:HEM:HBD1	1.81	0.63
2:C:601:HEM:HBC2	2:C:601:HEM:HMC1	1.82	0.62
2:D:601:HEM:HMC1	2:D:601:HEM:HBC2	1.81	0.62
1:D:49:ILE:HD12	1:D:53:LEU:HD23	1.82	0.61
1:B:237:ILE:HB	1:B:240:LEU:HD12	1.82	0.61
1:D:191:VAL:O	1:D:195:THR:OG1	2.07	0.61
1:C:440:ASP:OD1	1:C:442:VAL:HG12	1.99	0.61
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.83	0.61
1:A:174:LEU:HD22	1:A:184:PHE:CE2	2.36	0.60
1:D:478:VAL:HG13	1:D:508:MET:HG3	1.82	0.60
1:B:299:ASN:O	1:B:300:VAL:HB	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASP:HA	3:A:602:KUV:C1	2.31	0.60
1:B:334:VAL:HG21	1:B:506:PHE:CE2	2.37	0.60
2:D:601:HEM:HBD1	2:D:601:HEM:HHA	1.83	0.59
1:D:46:TRP:O	1:D:77:ARG:NH2	2.36	0.58
1:D:162:HIS:CB	1:D:197:VAL:HG23	2.34	0.57
1:D:162:HIS:HB3	1:D:197:VAL:HG23	1.86	0.57
1:A:343:ILE:HD11	1:A:368:MET:HE2	1.87	0.57
1:D:134:ARG:O	1:D:137:LEU:N	2.37	0.56
1:B:347:LEU:HD23	1:B:365:LEU:CD2	2.36	0.56
1:A:343:ILE:HD11	1:A:368:MET:CE	2.35	0.56
1:A:262:MET:O	1:A:266:VAL:HG23	2.05	0.56
1:A:369:GLU:O	1:A:373:LEU:HG	2.06	0.56
1:C:368:MET:O	1:C:372:ILE:HD12	2.06	0.56
1:D:359:LEU:HD13	1:D:359:LEU:O	2.06	0.56
2:B:601:HEM:HBD1	2:B:601:HEM:HHA	1.88	0.55
1:D:95:ALA:HB2	1:D:396:LEU:HD22	1.88	0.55
1:A:207:TYR:CD2	1:A:214:LEU:HD13	2.42	0.55
1:D:150:ASP:HB3	1:D:151:PRO:CD	2.37	0.55
1:D:109:LEU:HD12	1:D:112:PHE:CE2	2.42	0.55
1:B:455:ARG:NH1	2:B:601:HEM:O2D	2.40	0.54
1:B:171:ILE:HD13	1:B:477:ARG:NH2	2.22	0.54
1:D:63:LEU:HD12	1:D:384:PHE:CZ	2.42	0.54
1:D:163:VAL:HG11	1:D:469:LEU:HB3	1.89	0.53
1:D:173:THR:O	1:D:177:LEU:HD12	2.09	0.53
1:A:187:TYR:O	1:A:191:VAL:HG12	2.09	0.53
1:D:308:ILE:O	1:D:311:VAL:HG12	2.08	0.53
1:A:159:LEU:O	1:A:163:VAL:HG23	2.09	0.53
1:B:460:GLU:OE2	1:B:464:ARG:NH1	2.41	0.53
1:D:327:SER:OG	1:D:500:HIS:NE2	2.41	0.53
2:D:601:HEM:CBD	2:D:601:HEM:HHA	2.39	0.53
1:D:150:ASP:HB3	1:D:151:PRO:HD2	1.89	0.53
1:D:374:GLU:OE1	1:D:377:ARG:NE	2.36	0.53
1:D:191:VAL:HG22	1:D:218:VAL:HG21	1.92	0.52
1:A:374:GLU:OE2	1:A:431:ARG:NH1	2.43	0.52
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.92	0.51
1:D:78:ILE:HG21	1:D:236:PHE:HD2	1.75	0.51
1:A:186:PRO:O	1:A:190:VAL:HG23	2.10	0.51
1:C:114:LEU:HD22	1:C:252:LYS:HG3	1.91	0.51
1:C:422:VAL:HG23	1:C:423:ASN:H	1.76	0.51
1:D:410:ASN:OD1	1:D:413:GLN:N	2.41	0.51
1:A:382:VAL:HG21	2:A:601:HEM:HMB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:VAL:HG21	1:D:308:ILE:HG21	1.93	0.51
1:D:422:VAL:HG23	1:D:423:ASN:H	1.76	0.51
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.93	0.51
1:A:237:ILE:HG22	1:A:239:ILE:HG22	1.93	0.50
1:A:272:THR:O	1:A:279:ARG:NH2	2.44	0.50
1:A:478:VAL:HG11	1:A:480:PHE:CZ	2.46	0.50
1:C:374:GLU:HA	1:C:374:GLU:OE1	2.10	0.50
1:B:195:THR:HG21	1:B:214:LEU:HD11	1.93	0.50
1:D:41:PRO:HD3	1:D:399:PHE:CE2	2.47	0.50
1:D:422:VAL:HG23	1:D:423:ASN:N	2.26	0.49
1:B:262:MET:O	1:B:266:VAL:HG23	2.12	0.49
1:C:150:ASP:O	1:C:152:ALA:N	2.45	0.49
1:C:335:MET:HE3	1:C:488:VAL:HG11	1.94	0.49
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.43	0.49
2:C:601:HEM:HBC2	2:C:601:HEM:CMC	2.42	0.49
1:D:343:ILE:HD11	1:D:368:MET:CE	2.43	0.49
2:D:601:HEM:HBC2	2:D:601:HEM:CMC	2.42	0.49
1:B:422:VAL:HG23	1:B:423:ASN:H	1.77	0.49
1:C:355:ARG:NH2	1:C:361:ASP:OD2	2.46	0.49
2:A:601:HEM:HBC2	2:A:601:HEM:HMC1	1.94	0.49
2:C:601:HEM:HHA	2:C:601:HEM:CBD	2.43	0.49
1:C:334:VAL:HG21	1:C:506:PHE:CE2	2.47	0.49
1:C:142:LEU:HB3	1:C:462:ILE:HD11	1.94	0.49
1:D:150:ASP:O	1:D:152:ALA:N	2.46	0.49
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.42	0.49
1:C:240:LEU:HD23	1:C:243:LEU:HD12	1.95	0.48
1:A:164:SER:CB	1:A:356:ARG:HH22	2.26	0.48
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.44	0.48
1:A:388:HIS:NE2	2:A:601:HEM:O1A	2.41	0.48
1:A:336:ASN:O	1:A:336:ASN:ND2	2.46	0.48
1:B:186:PRO:O	1:B:190:VAL:HG23	2.13	0.48
2:B:601:HEM:CMB	2:B:601:HEM:HBB2	2.44	0.48
1:C:305:GLU:O	1:C:309:ASN:HB3	2.12	0.48
1:D:334:VAL:HG21	1:D:506:PHE:CE2	2.48	0.48
1:C:131:TRP:CZ2	1:C:135:ARG:HD3	2.49	0.48
1:B:274:GLU:HB2	1:B:277:HIS:HB3	1.95	0.48
1:D:188:ARG:O	1:D:191:VAL:HG12	2.13	0.48
1:A:111:THR:HG23	1:A:235:ASP:OD1	2.14	0.47
1:C:237:ILE:HB	1:C:240:LEU:HD12	1.96	0.47
1:C:86:LEU:O	1:C:92:ILE:HD11	2.13	0.47
1:D:150:ASP:CB	1:D:151:PRO:CD	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG21	1:A:251:PHE:CG	2.49	0.47
1:A:301:GLN:OE1	1:A:302:LEU:N	2.46	0.47
1:A:278:ILE:HG23	1:A:283:ASP:HB3	1.94	0.47
1:C:211:HIS:O	1:C:215:LEU:HD12	2.15	0.47
1:D:191:VAL:HG22	1:D:218:VAL:CG2	2.44	0.47
1:A:449:ILE:HG23	1:A:450:PHE:CD1	2.50	0.47
1:A:216:SER:HA	1:A:220:LEU:HB2	1.96	0.47
1:A:339:VAL:O	1:A:343:ILE:HG22	2.13	0.47
2:A:601:HEM:HBD1	2:A:601:HEM:HHA	1.96	0.47
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.96	0.46
1:B:183:HIS:O	1:B:183:HIS:ND1	2.45	0.46
1:D:147:ILE:HD11	1:D:465:TRP:CZ3	2.50	0.46
1:A:361:ASP:O	1:A:365:LEU:HD12	2.14	0.46
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.97	0.46
3:A:602:KUV:C1	3:A:602:KUV:C32	2.93	0.46
1:D:254:LEU:HD23	1:D:254:LEU:C	2.36	0.46
1:B:343:ILE:HG21	1:B:475:LEU:HD13	1.97	0.46
1:C:159:LEU:O	1:C:163:VAL:HG23	2.15	0.46
1:D:177:LEU:HD21	1:D:189:TYR:OH	2.15	0.46
1:B:309:ASN:OD1	1:B:309:ASN:C	2.54	0.46
1:C:192:VAL:HG11	1:C:209:HIS:HA	1.98	0.45
1:D:334:VAL:HG11	1:D:482:VAL:HB	1.98	0.45
1:A:224:PHE:HD1	1:A:226:GLU:H	1.64	0.45
1:B:187:TYR:O	1:B:191:VAL:HG12	2.17	0.45
1:B:484:LEU:HD23	1:B:485:GLY:N	2.31	0.45
1:C:150:ASP:HB3	1:C:158:TYR:CZ	2.50	0.45
1:D:336:ASN:ND2	1:D:336:ASN:O	2.48	0.45
1:B:430:GLU:N	1:B:430:GLU:OE1	2.48	0.45
1:B:415:ASN:ND2	1:B:448:ILE:O	2.43	0.45
1:B:456:LYS:NZ	1:B:460:GLU:OE1	2.37	0.45
1:C:213:GLU:OE1	1:C:264:LYS:NZ	2.49	0.45
1:A:166:GLU:HG2	1:A:193:SER:HA	1.99	0.45
1:C:175:GLN:HE21	1:C:510:LEU:HD11	1.81	0.45
1:C:478:VAL:HG13	1:C:508:MET:HG3	1.99	0.45
1:D:456:LYS:NZ	1:D:460:GLU:OE1	2.41	0.45
1:A:265:MET:O	1:A:269:HIS:ND1	2.50	0.45
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	1.99	0.45
1:B:434:THR:HB	1:B:435:PRO:CD	2.48	0.45
1:D:63:LEU:HD12	1:D:384:PHE:HZ	1.81	0.44
1:B:63:LEU:HD22	1:B:85:VAL:HG21	1.99	0.44
1:D:343:ILE:HD11	1:D:368:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:LEU:O	1:C:431:ARG:HG2	2.18	0.44
1:D:227:VAL:HG11	1:D:251:PHE:CG	2.52	0.44
1:C:308:ILE:O	1:C:311:VAL:HG12	2.18	0.44
1:B:72:ASP:HB3	1:B:91:THR:HG21	1.99	0.44
1:D:194:VAL:O	1:D:197:VAL:HG12	2.18	0.44
1:A:221:ASN:O	1:A:222:ASN:C	2.55	0.44
1:D:388:HIS:HE1	1:D:455:ARG:HB2	1.83	0.43
1:A:458:ILE:HD11	2:A:601:HEM:HMD2	2.00	0.43
1:C:245:ASN:HB3	1:C:248:LEU:HB3	1.99	0.43
1:C:72:ASP:CB	1:C:91:THR:HG21	2.47	0.43
1:D:337:PRO:HA	1:D:340:GLN:HB2	1.99	0.43
1:A:38:LYS:O	1:A:399:PHE:HA	2.19	0.43
1:B:440:ASP:OD1	1:B:442:VAL:HG12	2.19	0.43
1:B:49:ILE:HD12	1:B:53:LEU:HD23	2.00	0.43
1:C:72:ASP:HB3	1:C:91:THR:HG21	2.00	0.43
1:D:70:TYR:CD1	1:D:70:TYR:N	2.87	0.43
1:A:223:ASN:HB2	3:A:602:KUV:C18	2.49	0.42
1:C:344:GLN:OE1	1:C:511:ARG:NH1	2.52	0.42
1:D:413:GLN:O	1:D:417:ASP:N	2.53	0.42
1:A:334:VAL:HG21	1:A:506:PHE:CD2	2.54	0.42
1:C:335:MET:HE1	1:C:488:VAL:HG21	2.02	0.42
1:A:377:ARG:O	1:A:380:SER:OG	2.25	0.42
1:C:343:ILE:O	1:C:347:LEU:HG	2.19	0.42
1:D:218:VAL:HG23	1:D:319:PHE:CD1	2.55	0.42
1:B:374:GLU:OE2	1:B:377:ARG:NH2	2.43	0.42
1:A:112:PHE:N	1:A:112:PHE:CD1	2.87	0.41
1:D:468:PHE:CD1	1:D:469:LEU:N	2.88	0.41
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.50	0.41
1:C:374:GLU:OE2	1:C:431:ARG:NH1	2.50	0.41
1:D:150:ASP:CG	1:D:151:PRO:HD3	2.41	0.41
1:A:463:ALA:O	1:A:467:VAL:HG23	2.20	0.41
1:B:462:ILE:O	1:B:466:GLU:HB2	2.21	0.41
1:C:325:ALA:HB2	1:C:381:PHE:CZ	2.55	0.41
1:D:218:VAL:HG23	1:D:319:PHE:CE1	2.55	0.41
1:B:477:ARG:O	1:B:478:VAL:HG23	2.21	0.41
1:B:494:TYR:CG	1:B:495:GLY:N	2.89	0.41
1:D:374:GLU:OE1	1:D:374:GLU:HA	2.20	0.41
1:C:335:MET:O	1:C:337:PRO:HD3	2.20	0.41
1:B:434:THR:HB	1:B:435:PRO:HD2	2.03	0.41
1:C:222:ASN:OD1	1:C:222:ASN:O	2.39	0.41
1:C:237:ILE:HG22	1:C:239:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PRO:O	1:D:51:HIS:NE2	2.42	0.41
1:A:160:GLU:OE2	1:A:358:ARG:CG	2.68	0.41
1:A:190:VAL:O	1:A:194:VAL:HG23	2.21	0.41
1:B:164:SER:OG	1:B:356:ARG:NH1	2.53	0.41
1:A:92:ILE:HG23	1:A:96:LEU:HD12	2.03	0.41
1:D:135:ARG:NH2	1:D:456:LYS:O	2.51	0.41
1:C:223:ASN:O	1:C:224:PHE:C	2.58	0.41
1:D:361:ASP:O	1:D:365:LEU:HD12	2.21	0.41
1:A:133:ALA:O	1:A:137:LEU:HG	2.21	0.41
1:A:131:TRP:CZ2	1:A:135:ARG:HD3	2.56	0.41
1:D:93:ARG:HG3	1:D:97:VAL:HG21	2.02	0.41
1:A:163:VAL:HG13	1:A:470:PHE:CE2	2.56	0.40
1:B:194:VAL:HG13	1:B:466:GLU:OE1	2.21	0.40
1:D:197:VAL:HG11	1:D:466:GLU:OE1	2.21	0.40
1:B:302:LEU:HD22	1:B:307:ILE:HG12	2.04	0.40
1:C:374:GLU:OE1	1:C:377:ARG:NE	2.42	0.40
1:A:337:PRO:HA	1:A:340:GLN:HB2	2.03	0.40
1:A:428:LEU:O	1:A:431:ARG:HG2	2.21	0.40
1:B:211:HIS:HE1	1:B:213:GLU:HB3	1.87	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	458/491 (93%)	430 (94%)	25 (6%)	3 (1%)	22 60
1	B	466/491 (95%)	435 (93%)	29 (6%)	2 (0%)	34 69
1	C	464/491 (94%)	421 (91%)	40 (9%)	3 (1%)	25 63
1	D	452/491 (92%)	415 (92%)	32 (7%)	5 (1%)	14 50
All	All	1840/1964 (94%)	1701 (92%)	126 (7%)	13 (1%)	22 60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	VAL
1	D	150	ASP
1	D	351	ILE
1	A	222	ASN
1	A	449	ILE
1	B	449	ILE
1	D	148	ALA
1	D	88	GLY
1	C	225	GLY
1	C	151	PRO
1	C	449	ILE
1	A	88	GLY
1	D	449	ILE

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	415/439 (94%)	405 (98%)	10 (2%)	49	76
1	B	421/439 (96%)	416 (99%)	5 (1%)	71	87
1	C	418/439 (95%)	409 (98%)	9 (2%)	52	78
1	D	409/439 (93%)	397 (97%)	12 (3%)	42	72
All	All	1663/1756 (95%)	1627 (98%)	36 (2%)	52	78

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	90	ASP
1	A	101	ASP
1	A	206	ARG
1	A	224	PHE
1	A	301	GLN
1	A	336	ASN

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Mol	Chain	Res	Type
1	A	341	ARG
1	A	464	ARG
1	A	468	PHE
1	B	74	LEU
1	B	158	TYR
1	B	259	TYR
1	B	353	ARG
1	B	464	ARG
1	C	74	LEU
1	C	153	SER
1	C	221	ASN
1	C	223	ASN
1	C	224	PHE
1	C	245	ASN
1	C	259	TYR
1	C	288	HIS
1	C	336	ASN
1	D	74	LEU
1	D	101	ASP
1	D	149	SER
1	D	219	ASN
1	D	223	ASN
1	D	224	PHE
1	D	258	PHE
1	D	269	HIS
1	D	313	ASP
1	D	336	ASN
1	D	395	SER
1	D	468	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
2	HEM	C	601	-	27,50,50	1.85	5 (18%)	17,82,82	1.61	3 (17%)
2	HEM	A	601	-	27,50,50	1.84	4 (14%)	17,82,82	1.77	5 (29%)
2	HEM	D	601	-	27,50,50	1.85	4 (14%)	17,82,82	1.74	5 (29%)
3	KUV	A	602	-	27,35,35	2.97	12 (44%)	19,51,51	2.85	8 (42%)
4	NO3	B	602	-	1,3,3	0.61	0	0,3,3	0.00	-
2	HEM	B	601	1	27,50,50	1.83	4 (14%)	17,82,82	1.89	5 (29%)

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	-	-	4/6/54/54	-
3	KUV	A	602	-	-	0/2/30/30	0/4/4/4
2	HEM	D	601	-	-	4/6/54/54	-
2	HEM	C	601	-	-	3/6/54/54	-
2	HEM	B	601	1	-	4/6/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	KUV	C13-S12	6.63	1.82	1.73
3	A	602	KUV	C5-C4	5.58	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	KUV	C11-S12	5.52	1.81	1.72
3	A	602	KUV	C31-C32	5.33	1.61	1.52
3	A	602	KUV	C1-N2	-5.20	1.37	1.47
2	A	601	HEM	C3B-C2B	-4.27	1.34	1.40
2	B	601	HEM	C3B-C2B	-4.23	1.34	1.40
2	B	601	HEM	C3C-C2C	-4.19	1.34	1.40
2	A	601	HEM	C3C-C2C	-4.19	1.34	1.40
2	D	601	HEM	C3B-C2B	-4.14	1.34	1.40
2	C	601	HEM	C3B-C2B	-4.08	1.34	1.40
2	D	601	HEM	C3C-C2C	-4.08	1.34	1.40
3	A	602	KUV	C32-N24	4.00	1.51	1.46
2	C	601	HEM	C3C-C2C	-3.95	1.34	1.40
2	D	601	HEM	C3C-CAC	3.73	1.55	1.47
2	C	601	HEM	C3C-CAC	3.73	1.55	1.47
2	C	601	HEM	C3B-CAB	3.51	1.55	1.47
2	A	601	HEM	C3C-CAC	3.49	1.55	1.47
2	A	601	HEM	C3B-CAB	3.48	1.55	1.47
2	D	601	HEM	C3B-CAB	3.48	1.55	1.47
2	B	601	HEM	C3B-CAB	3.47	1.55	1.47
2	B	601	HEM	C3C-CAC	3.30	1.54	1.47
3	A	602	KUV	C25-N24	3.18	1.50	1.46
3	A	602	KUV	C8-N7	3.12	1.44	1.35
3	A	602	KUV	C15-C20	2.75	1.43	1.39
3	A	602	KUV	C15-C16	2.64	1.43	1.39
3	A	602	KUV	C13-N14	2.14	1.34	1.31
2	C	601	HEM	CAD-C3D	2.03	1.55	1.52
3	A	602	KUV	C26-C25	2.01	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	KUV	C20-C15-C16	-6.23	108.44	114.56
3	A	602	KUV	C31-C32-N24	5.79	123.46	113.48
3	A	602	KUV	C26-C25-N24	4.56	121.34	113.48
3	A	602	KUV	C16-C15-C13	3.87	127.69	121.78
2	B	601	HEM	CAA-CBA-CGA	-3.67	106.51	112.67
2	C	601	HEM	CMD-C2D-C1D	-3.65	122.86	128.46
2	D	601	HEM	CAA-CBA-CGA	-3.64	106.57	112.67
2	A	601	HEM	CAA-CBA-CGA	-3.33	107.08	112.67
2	B	601	HEM	CBD-CAD-C3D	-3.08	106.81	112.48
2	A	601	HEM	CMA-C3A-C4A	-3.00	123.85	128.46
2	B	601	HEM	CMD-C2D-C1D	-2.91	123.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	KUV	C17-C16-C15	2.81	127.37	123.94
2	D	601	HEM	CMD-C2D-C1D	-2.71	124.29	128.46
3	A	602	KUV	O9-C8-N7	-2.67	117.61	123.71
2	A	601	HEM	CAD-CBD-CGD	-2.46	108.54	112.67
2	B	601	HEM	CMA-C3A-C4A	-2.44	124.71	128.46
2	D	601	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
3	A	602	KUV	C19-C20-C15	2.35	126.80	123.94
2	B	601	HEM	CMC-C2C-C3C	2.32	129.01	124.68
3	A	602	KUV	C5-N6-N2	2.29	106.61	104.23
2	C	601	HEM	CAA-CBA-CGA	-2.28	108.85	112.67
2	C	601	HEM	C1D-C2D-C3D	2.23	108.55	107.00
2	A	601	HEM	CMD-C2D-C1D	-2.22	125.06	128.46
2	D	601	HEM	CAD-CBD-CGD	-2.17	109.03	112.67
2	A	601	HEM	CMC-C2C-C3C	2.17	128.74	124.68
2	D	601	HEM	CMB-C2B-C3B	2.15	128.70	124.68

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	C2D-C3D-CAD-CBD
2	C	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	C1A-C2A-CAA-CBA
2	A	601	HEM	C3A-C2A-CAA-CBA
2	A	601	HEM	C2D-C3D-CAD-CBD
2	A	601	HEM	C4D-C3D-CAD-CBD
2	D	601	HEM	C1A-C2A-CAA-CBA
2	D	601	HEM	C3A-C2A-CAA-CBA
2	D	601	HEM	C2D-C3D-CAD-CBD
2	D	601	HEM	C4D-C3D-CAD-CBD
2	B	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C3A-C2A-CAA-CBA
2	C	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C2D-C3D-CAD-CBD
2	B	601	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

5 monomers are involved in 28 short contacts:

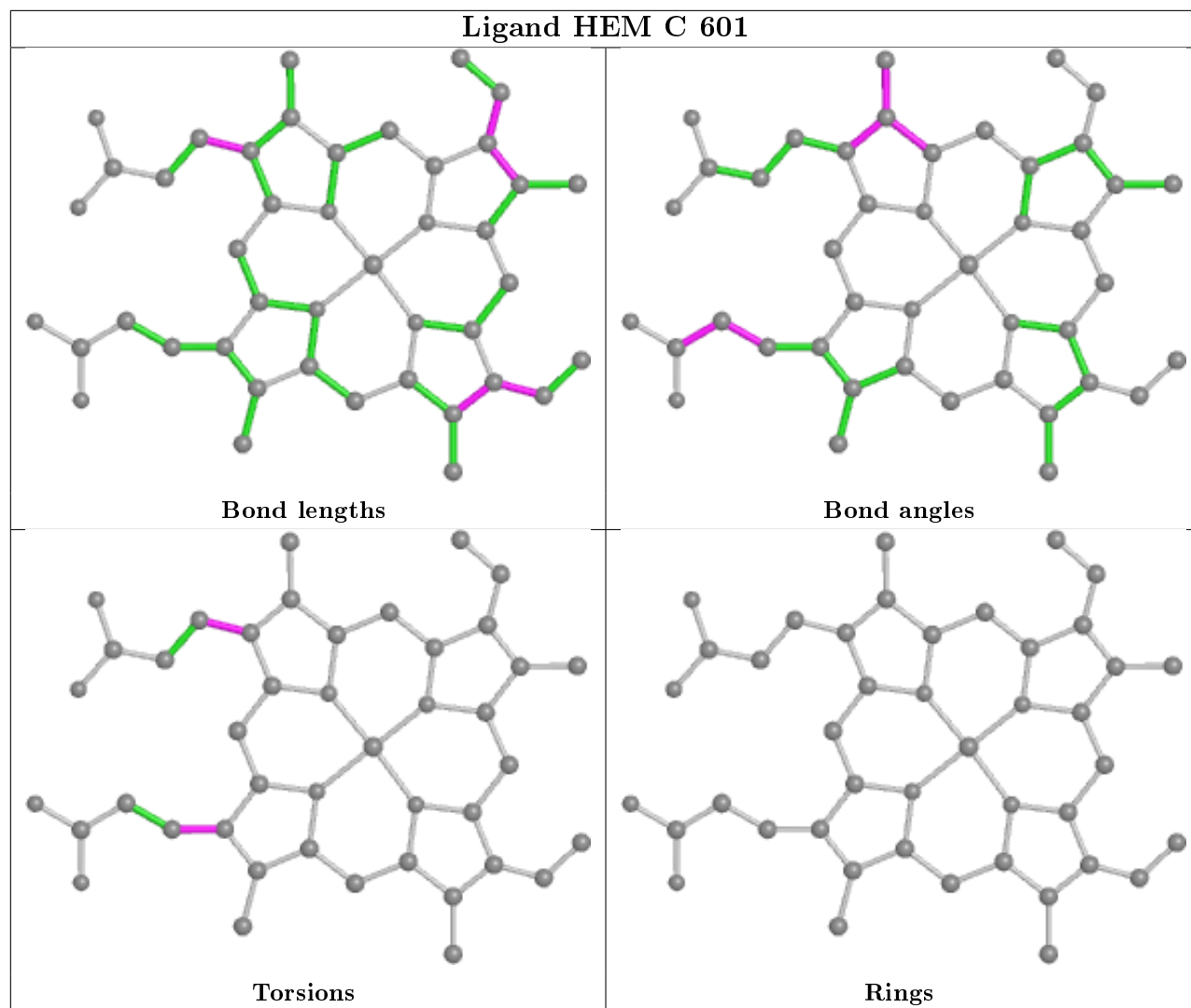
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	6	0

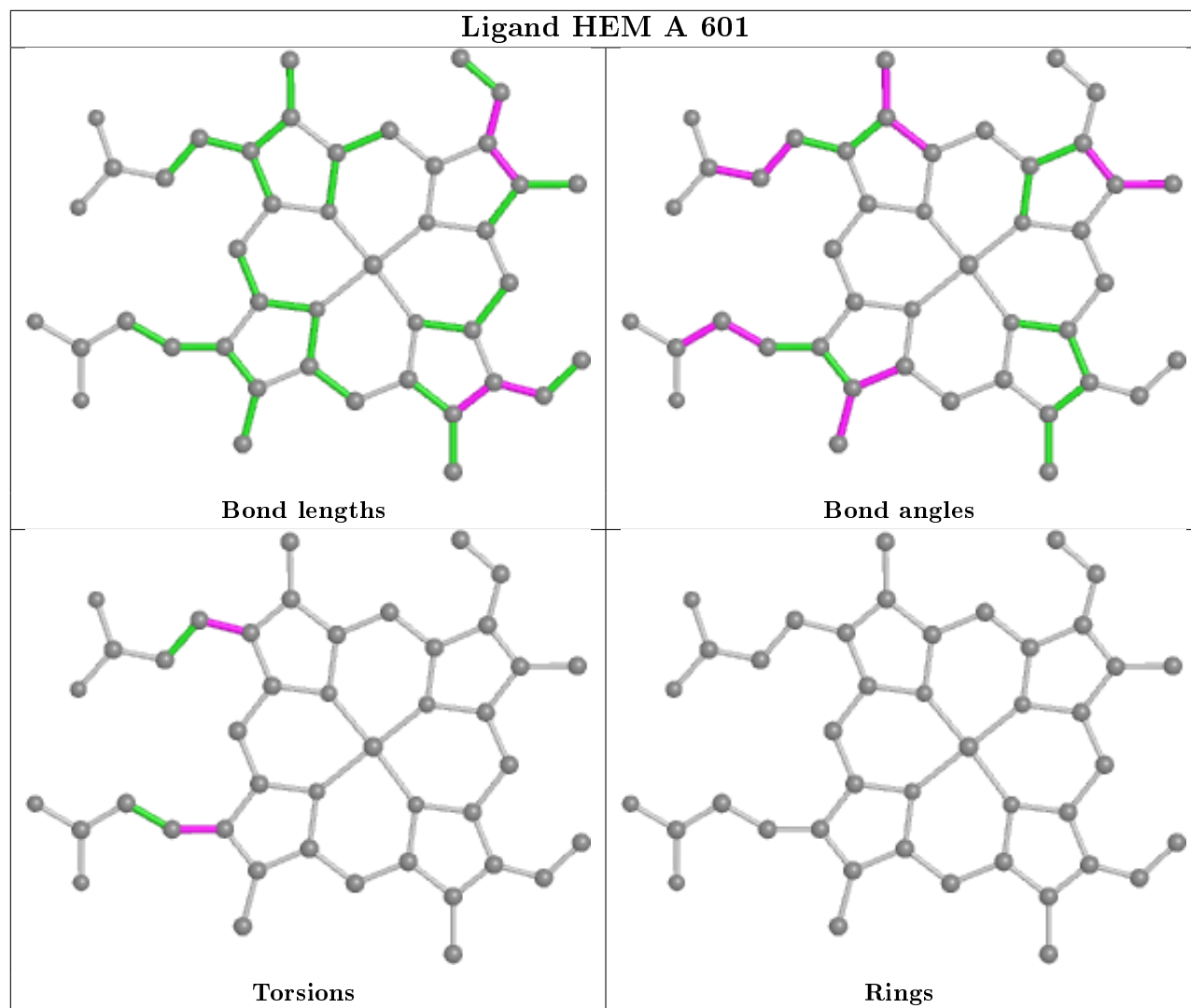
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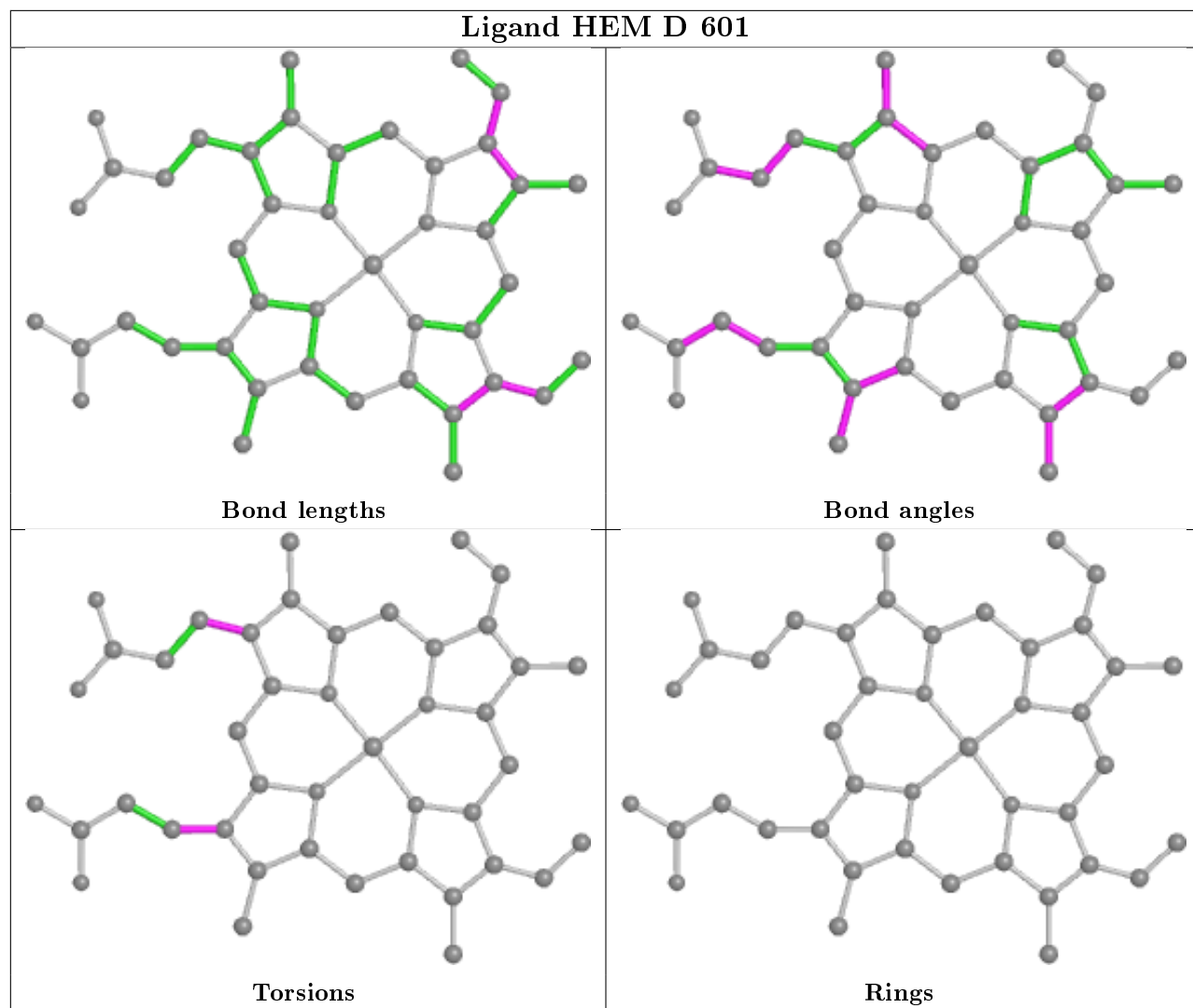
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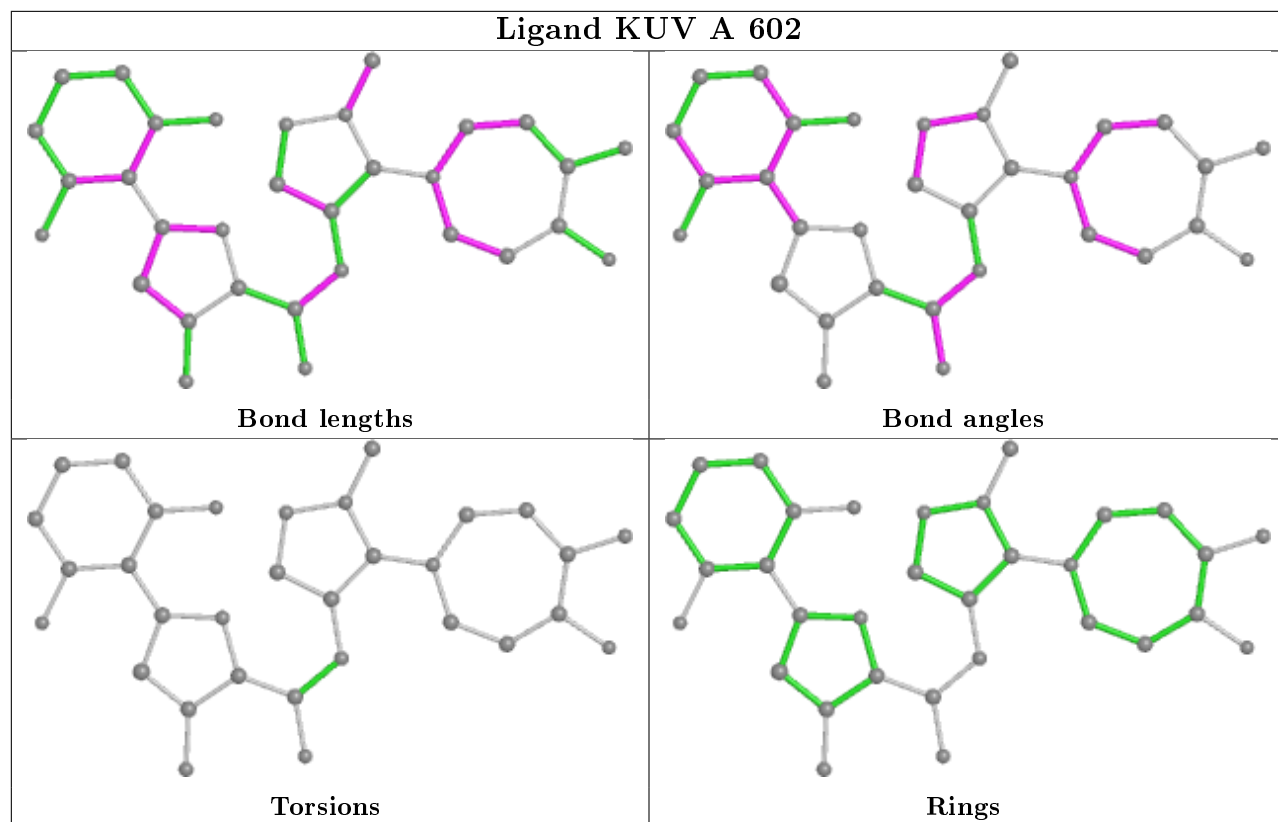
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	9	0
2	D	601	HEM	6	0
3	A	602	KUV	3	0
2	B	601	HEM	4	0

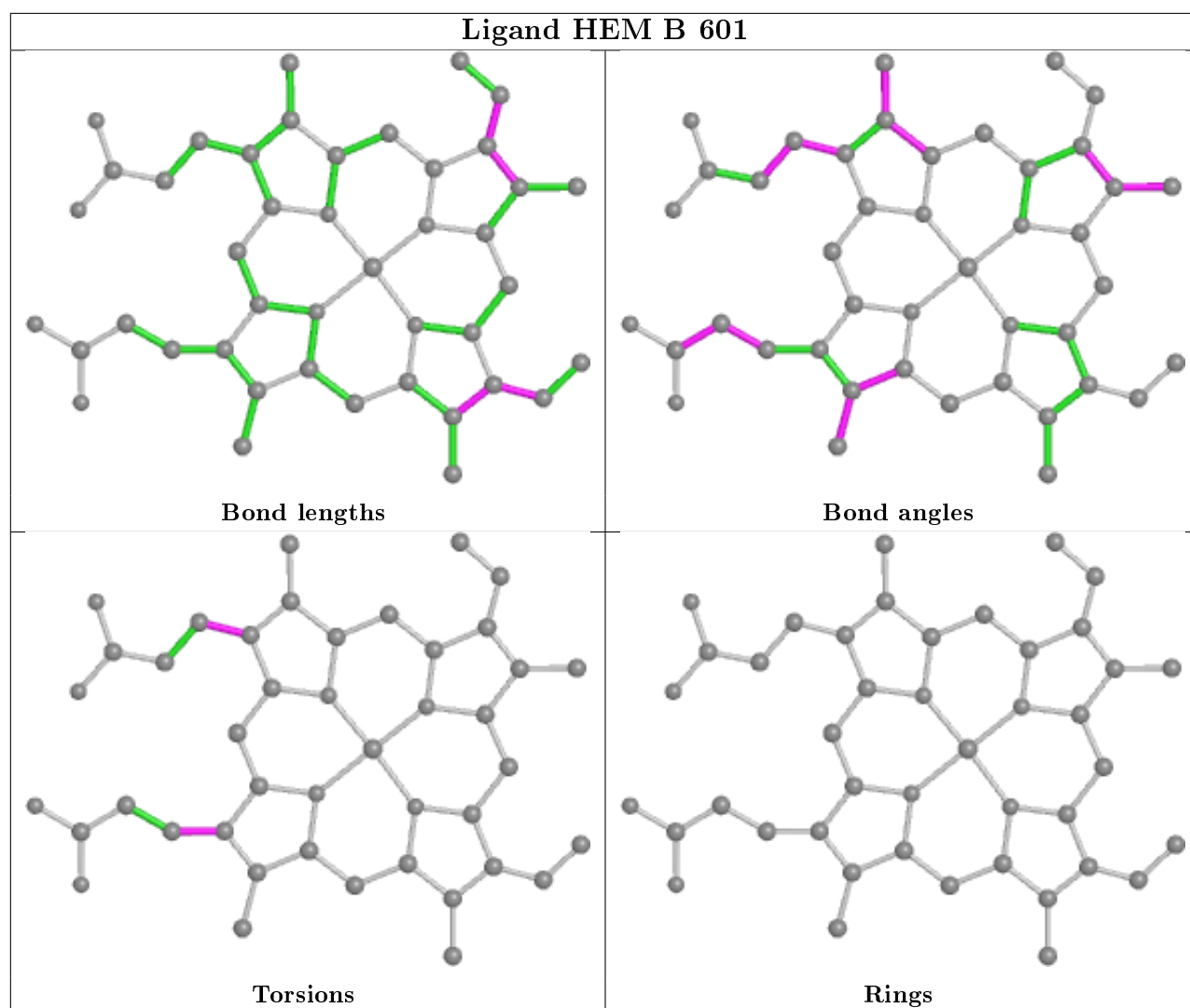
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	464/491 (94%)	0.27	3 (0%) 89 83	49, 71, 96, 120	0
1	B	470/491 (95%)	0.29	5 (1%) 80 69	48, 63, 82, 97	0
1	C	468/491 (95%)	0.34	15 (3%) 47 31	66, 91, 113, 121	0
1	D	458/491 (93%)	0.43	16 (3%) 44 28	72, 97, 112, 121	0
All	All	1860/1964 (94%)	0.33	39 (2%) 63 49	48, 81, 109, 121	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	GLU	4.4
1	C	289	CYS	3.4
1	B	221	ASN	3.2
1	C	153	SER	3.0
1	D	351	ILE	2.9
1	C	155	THR	2.8
1	D	73	VAL	2.7
1	D	476	GLN	2.7
1	D	364	HIS	2.7
1	B	298	ALA	2.6
1	C	36	GLY	2.6
1	C	291	GLU	2.6
1	D	55	LEU	2.5
1	C	244	PRO	2.5
1	D	352	GLY	2.5
1	A	301	GLN	2.4
1	D	129	PRO	2.4
1	A	289	CYS	2.3
1	C	287	GLU	2.3
1	D	468	PHE	2.3
1	B	350	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	262	MET	2.3
1	C	290	GLN	2.3
1	D	512	SER	2.2
1	C	273	PHE	2.2
1	C	149	SER	2.2
1	D	354	SER	2.2
1	C	419	LYS	2.2
1	B	475	LEU	2.2
1	B	217	LEU	2.2
1	C	275	LYS	2.1
1	D	357	PRO	2.1
1	C	286	ILE	2.1
1	A	302	LEU	2.1
1	C	288	HIS	2.1
1	D	353	ARG	2.1
1	D	480	PHE	2.1
1	C	307	ILE	2.0
1	D	475	LEU	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 carbohydrates 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.

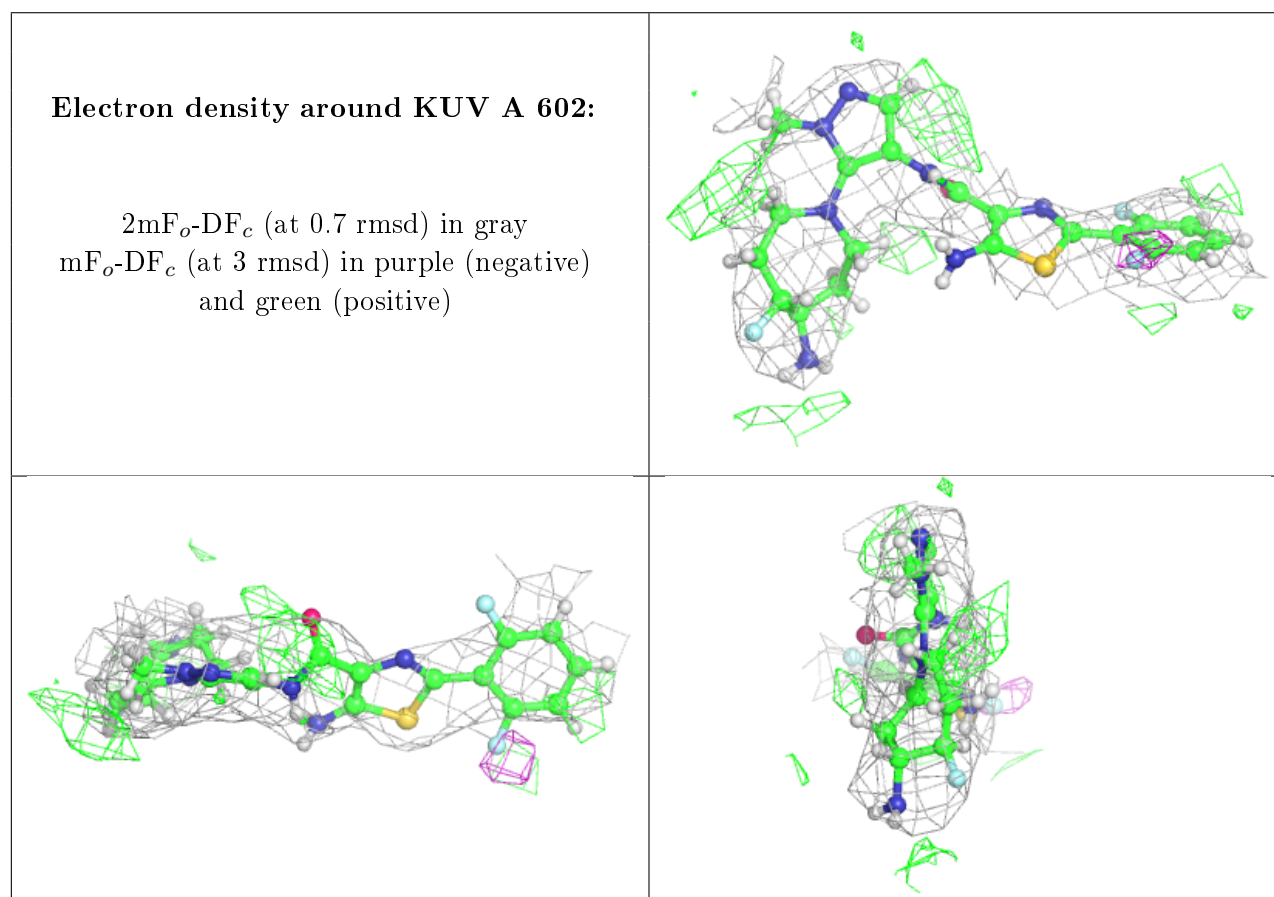
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	KUV	A	602	32/32	0.75	0.35	66,88,114,134	0
4	NO3	B	602	4/4	0.86	0.22	62,63,64,66	0
2	HEM	D	601	43/43	0.94	0.35	79,87,105,107	0
2	HEM	A	601	43/43	0.95	0.32	54,65,80,82	0
2	HEM	C	601	43/43	0.95	0.36	68,81,97,101	0

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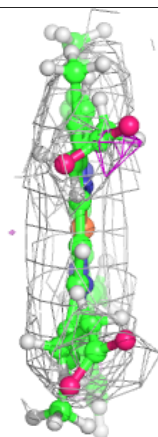
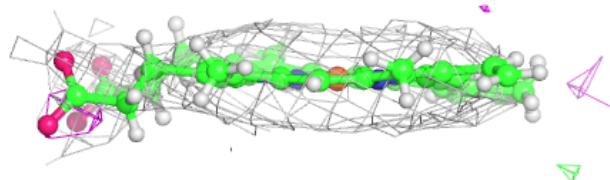
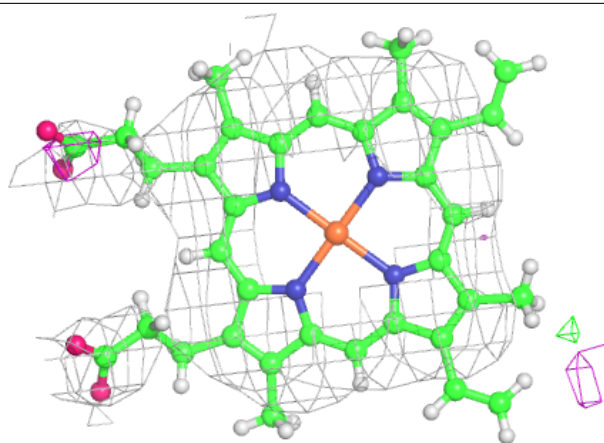
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	B	601	43/43	0.95	0.33	49,52,65,66	0

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.



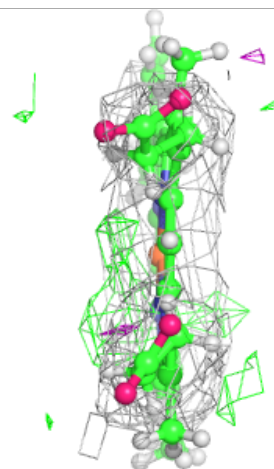
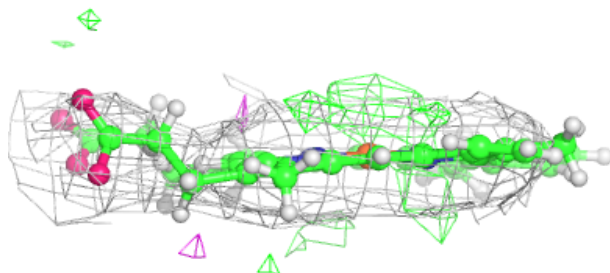
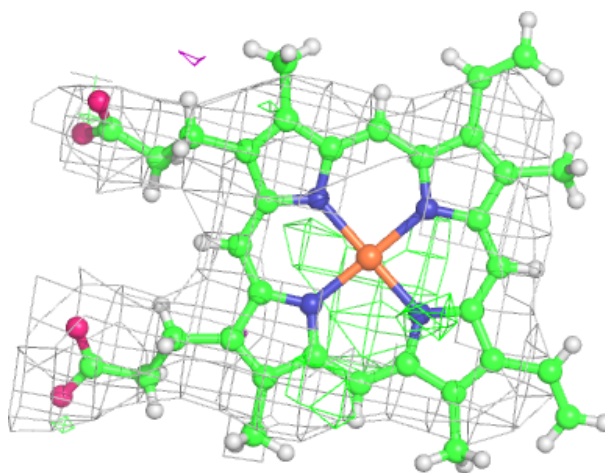
Electron density around HEM D 601:

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



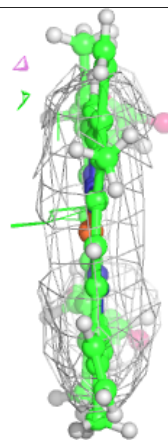
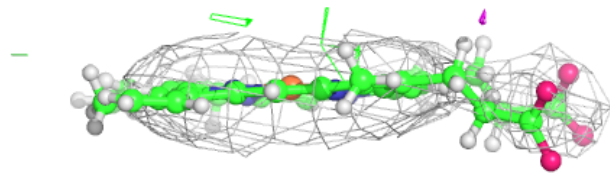
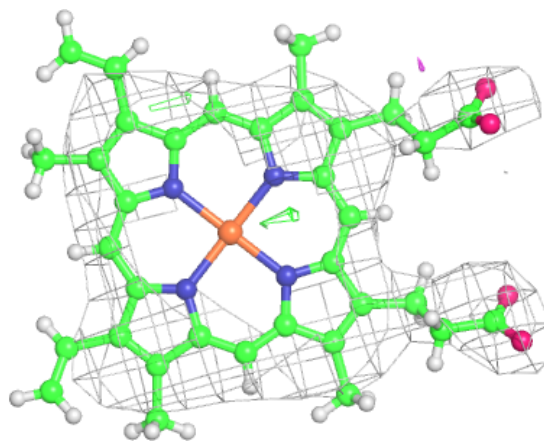
Electron density around HEM A 601:

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



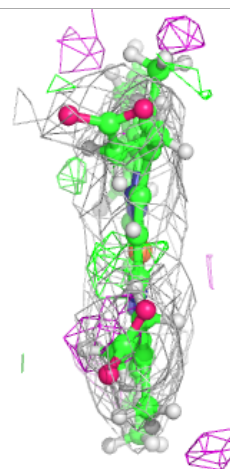
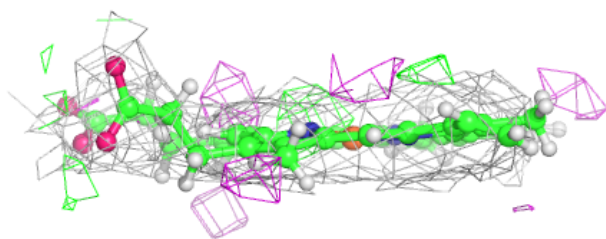
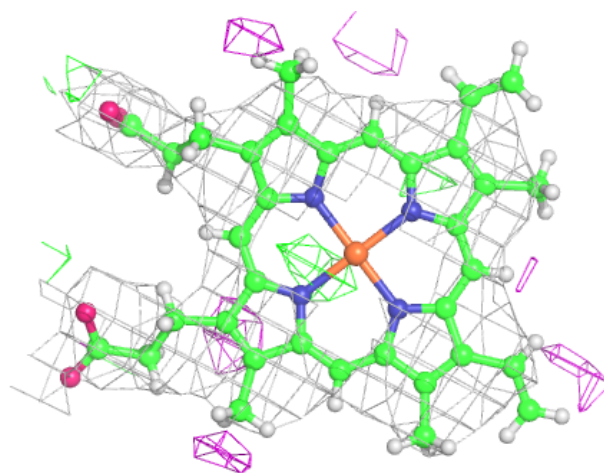
Electron density around HEM C 601:

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



Electron density around HEM B 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.