



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:24 PM BST

PDB ID : 6A4I
Title : Crystal Structure of human TDO inhibitor complex
Authors : Fu, G.; Wang, J.; Luo, G.; Wu, G.; Qian, K.
Deposited on : 2018-06-20
Resolution : 2.65 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 : 2.14.4.dev1
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) : 2.14.4.dev1

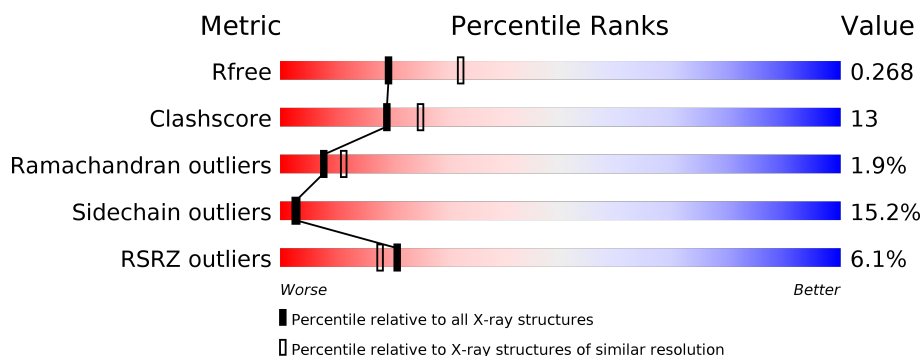
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	391	<div> <div>2%</div> <div>57%</div> <div>20%</div> <div>• •</div> <div>18%</div> </div>
1	B	391	<div> <div>4%</div> <div>50%</div> <div>21%</div> <div>8%</div> <div>•</div> <div>21%</div> </div>
1	C	391	<div> <div>6%</div> <div>53%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>17%</div> </div>
1	D	391	<div> <div>7%</div> <div>43%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>26%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10801 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2710	1745	469	485	11			
1	B	309	Total	C	N	O	S	0	0	0
			2608	1685	451	462	10			
1	C	323	Total	C	N	O	S	0	0	0
			2722	1751	479	481	11			
1	D	290	Total	C	N	O	S	0	1	0
			2463	1594	428	431	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P48775
A	-1	GLY	-	expression tag	UNP P48775
A	0	SER	-	expression tag	UNP P48775
A	1	SER	-	expression tag	UNP P48775
A	2	HIS	-	expression tag	UNP P48775
A	3	HIS	-	expression tag	UNP P48775
A	4	HIS	-	expression tag	UNP P48775
A	5	HIS	-	expression tag	UNP P48775
A	6	HIS	-	expression tag	UNP P48775
A	7	HIS	-	expression tag	UNP P48775
A	8	SER	-	expression tag	UNP P48775
A	9	SER	-	expression tag	UNP P48775
A	10	GLY	-	expression tag	UNP P48775
A	11	LEU	-	expression tag	UNP P48775
A	12	VAL	-	expression tag	UNP P48775
A	13	PRO	-	expression tag	UNP P48775
A	14	ARG	-	expression tag	UNP P48775
A	15	GLY	-	expression tag	UNP P48775
A	16	SER	-	expression tag	UNP P48775
A	17	HIS	-	expression tag	UNP P48775
A	18	MET	-	expression tag	UNP P48775

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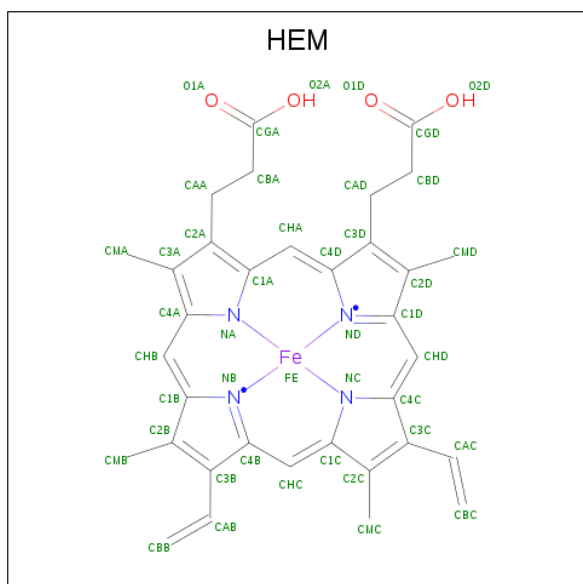
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P48775
B	-1	GLY	-	expression tag	UNP P48775
B	0	SER	-	expression tag	UNP P48775
B	1	SER	-	expression tag	UNP P48775
B	2	HIS	-	expression tag	UNP P48775
B	3	HIS	-	expression tag	UNP P48775
B	4	HIS	-	expression tag	UNP P48775
B	5	HIS	-	expression tag	UNP P48775
B	6	HIS	-	expression tag	UNP P48775
B	7	HIS	-	expression tag	UNP P48775
B	8	SER	-	expression tag	UNP P48775
B	9	SER	-	expression tag	UNP P48775
B	10	GLY	-	expression tag	UNP P48775
B	11	LEU	-	expression tag	UNP P48775
B	12	VAL	-	expression tag	UNP P48775
B	13	PRO	-	expression tag	UNP P48775
B	14	ARG	-	expression tag	UNP P48775
B	15	GLY	-	expression tag	UNP P48775
B	16	SER	-	expression tag	UNP P48775
B	17	HIS	-	expression tag	UNP P48775
B	18	MET	-	expression tag	UNP P48775
C	-2	MET	-	expression tag	UNP P48775
C	-1	GLY	-	expression tag	UNP P48775
C	0	SER	-	expression tag	UNP P48775
C	1	SER	-	expression tag	UNP P48775
C	2	HIS	-	expression tag	UNP P48775
C	3	HIS	-	expression tag	UNP P48775
C	4	HIS	-	expression tag	UNP P48775
C	5	HIS	-	expression tag	UNP P48775
C	6	HIS	-	expression tag	UNP P48775
C	7	HIS	-	expression tag	UNP P48775
C	8	SER	-	expression tag	UNP P48775
C	9	SER	-	expression tag	UNP P48775
C	10	GLY	-	expression tag	UNP P48775
C	11	LEU	-	expression tag	UNP P48775
C	12	VAL	-	expression tag	UNP P48775
C	13	PRO	-	expression tag	UNP P48775
C	14	ARG	-	expression tag	UNP P48775
C	15	GLY	-	expression tag	UNP P48775
C	16	SER	-	expression tag	UNP P48775
C	17	HIS	-	expression tag	UNP P48775
C	18	MET	-	expression tag	UNP P48775

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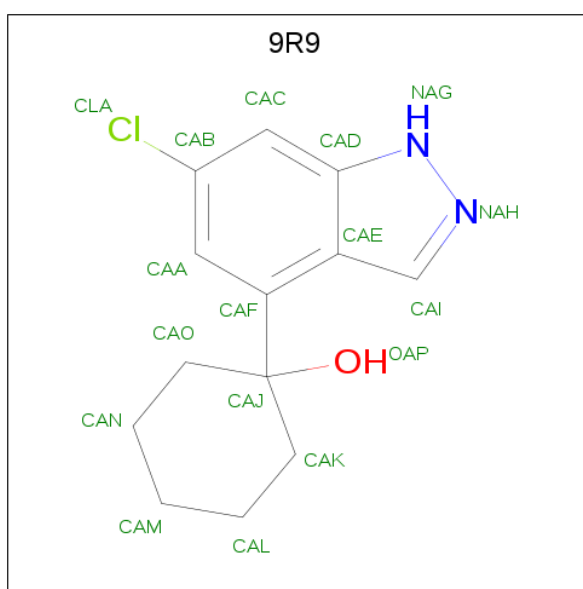
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP P48775
D	-1	GLY	-	expression tag	UNP P48775
D	0	SER	-	expression tag	UNP P48775
D	1	SER	-	expression tag	UNP P48775
D	2	HIS	-	expression tag	UNP P48775
D	3	HIS	-	expression tag	UNP P48775
D	4	HIS	-	expression tag	UNP P48775
D	5	HIS	-	expression tag	UNP P48775
D	6	HIS	-	expression tag	UNP P48775
D	7	HIS	-	expression tag	UNP P48775
D	8	SER	-	expression tag	UNP P48775
D	9	SER	-	expression tag	UNP P48775
D	10	GLY	-	expression tag	UNP P48775
D	11	LEU	-	expression tag	UNP P48775
D	12	VAL	-	expression tag	UNP P48775
D	13	PRO	-	expression tag	UNP P48775
D	14	ARG	-	expression tag	UNP P48775
D	15	GLY	-	expression tag	UNP P48775
D	16	SER	-	expression tag	UNP P48775
D	17	HIS	-	expression tag	UNP P48775
D	18	MET	-	expression tag	UNP P48775

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



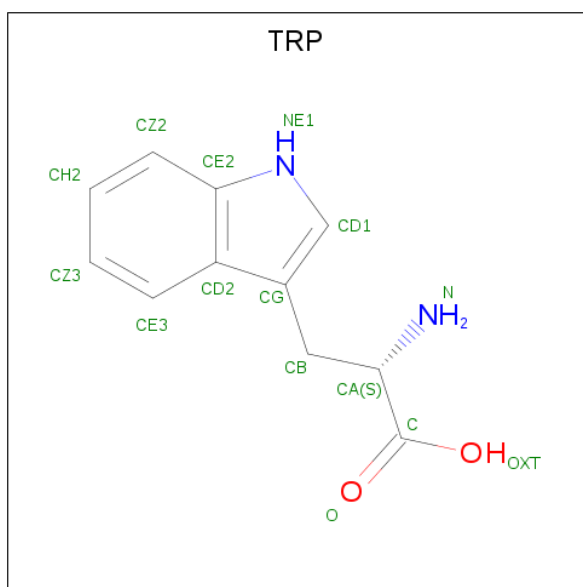
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-(6-chloro-1H-indazol-4-yl)cyclohexan-1-ol (three-letter code: 9R9) (formula: $C_{13}H_{15}ClN_2O$).



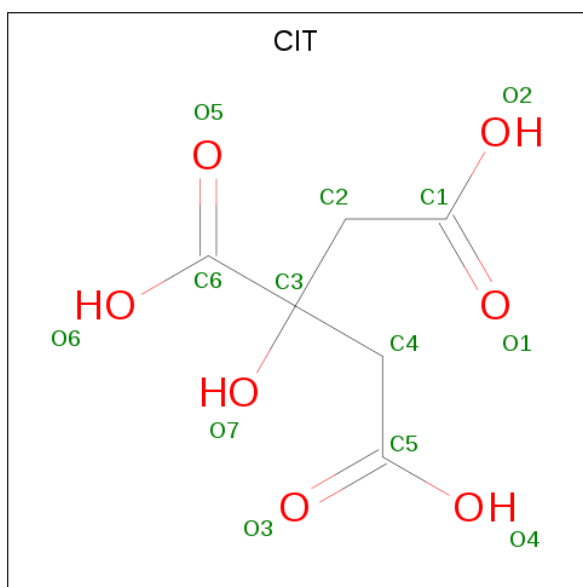
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
3	C	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
3	D	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		
4	D	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 29% 57% 20% 18%
- Chain A: MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS HIS MET PRO VAL GLY GLY GLY SER GLN THR VAL ASN ARG ARG ALA SER LYS GLY GLY L40 L41 N53 K65 H70 Y79 L90 D91 S92 E95 I96 E97

- Chain B:
-
- Amino Acid Composition Data (Estimated from Chart):
- | Amino Acid | Percentage (%) |
|------------|----------------|
| Met | 4% |
| Gly | 50% |
| Ser | 21% |
| His | 8% |
| Val | 21% |

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.31Å 144.11Å 89.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.17 – 2.65 48.04 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (106.17-2.65) 99.7 (48.04-2.64)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.205 , 0.269 0.205 , 0.268	Depositor DCC
R_{free} test set	3058 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10801	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CIT, 9R9

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	1.32	21/2769 (0.8%)	1.23	19/3723 (0.5%)
1	B	1.21	17/2668 (0.6%)	1.11	14/3592 (0.4%)
1	C	1.30	17/2782 (0.6%)	1.15	16/3743 (0.4%)
1	D	1.32	19/2521 (0.8%)	1.22	21/3395 (0.6%)
All	All	1.29	74/10740 (0.7%)	1.18	70/14453 (0.5%)

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	2
1	C	0	2
1	D	0	2
All	All	0	6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	GLU	N-CA	19.09	1.84	1.46
1	C	243	ALA	N-CA	16.20	1.78	1.46
1	D	286	TYR	CE1-CZ	15.53	1.58	1.38
1	C	227	GLU	CB-CG	14.52	1.79	1.52
1	C	232	ARG	CB-CG	13.79	1.89	1.52
1	D	286	TYR	CG-CD1	13.77	1.57	1.39
1	B	238	PHE	CG-CD1	13.68	1.59	1.38
1	B	236	GLU	CD-OE2	12.84	1.39	1.25
1	A	249	GLU	CG-CD	12.57	1.70	1.51
1	C	243	ALA	CA-C	-11.72	1.22	1.52
1	C	374	PRO	N-CD	11.17	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	GLU	CD-OE1	-11.12	1.13	1.25
1	C	235	GLU	CG-CD	-11.04	1.35	1.51
1	A	251	GLU	CD-OE2	10.46	1.37	1.25
1	C	236	GLU	CG-CD	8.97	1.65	1.51
1	D	282	ARG	NE-CZ	8.81	1.44	1.33
1	D	270	GLU	CD-OE2	8.71	1.35	1.25
1	A	243	ALA	C-O	8.51	1.39	1.23
1	C	377	TRP	CD2-CE2	-7.98	1.31	1.41
1	D	227	GLU	CD-OE1	7.86	1.34	1.25
1	D	274	GLU	C-O	7.54	1.37	1.23
1	B	236	GLU	CG-CD	7.50	1.63	1.51
1	A	248	GLU	CA-CB	-7.38	1.37	1.53
1	D	274	GLU	CD-OE2	7.35	1.33	1.25
1	C	377	TRP	CZ3-CH2	-7.22	1.28	1.40
1	D	274	GLU	CD-OE1	7.15	1.33	1.25
1	A	251	GLU	CB-CG	7.14	1.65	1.52
1	D	270	GLU	CA-C	7.03	1.71	1.52
1	B	233	GLY	N-CA	7.00	1.56	1.46
1	C	270	GLU	CD-OE2	6.96	1.33	1.25
1	A	95	GLU	CD-OE2	6.88	1.33	1.25
1	D	194	LYS	CD-CE	6.83	1.68	1.51
1	B	256	GLU	CD-OE1	6.81	1.33	1.25
1	B	257	PHE	CE2-CZ	6.81	1.50	1.37
1	D	189	ASN	CG-OD1	6.81	1.39	1.24
1	B	254	VAL	CA-CB	6.71	1.68	1.54
1	B	268	PHE	CE2-CZ	6.58	1.49	1.37
1	B	238	PHE	CE2-CZ	6.39	1.49	1.37
1	B	237	GLU	C-N	6.37	1.48	1.34
1	A	251	GLU	CD-OE1	-6.16	1.18	1.25
1	A	250	LYS	C-O	6.13	1.34	1.23
1	D	144	ARG	CZ-NH2	6.10	1.41	1.33
1	B	227	GLU	CB-CG	6.07	1.63	1.52
1	A	238	PHE	CG-CD1	5.77	1.47	1.38
1	C	233	GLY	N-CA	5.76	1.54	1.46
1	A	216	GLU	CG-CD	5.75	1.60	1.51
1	C	210	GLU	CB-CG	5.73	1.63	1.52
1	B	227	GLU	CD-OE2	5.73	1.31	1.25
1	D	185	LYS	C-O	5.73	1.34	1.23
1	A	216	GLU	CD-OE1	5.69	1.31	1.25
1	D	95	GLU	CD-OE1	5.63	1.31	1.25
1	D	210	GLU	CG-CD	5.63	1.60	1.51
1	A	250	LYS	N-CA	5.56	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	GLU	C-O	5.55	1.33	1.23
1	A	133	GLU	CD-OE1	5.54	1.31	1.25
1	C	296	TYR	CE1-CZ	5.50	1.45	1.38
1	D	271	LYS	N-CA	5.50	1.57	1.46
1	D	189	ASN	CG-ND2	5.49	1.46	1.32
1	A	301	GLU	CG-CD	5.48	1.60	1.51
1	C	239	ILE	CA-CB	5.47	1.67	1.54
1	A	95	GLU	CG-CD	5.44	1.60	1.51
1	A	249	GLU	CD-OE2	5.42	1.31	1.25
1	A	258	GLN	CG-CD	5.37	1.63	1.51
1	B	236	GLU	CD-OE1	5.37	1.31	1.25
1	B	256	GLU	CD-OE2	5.35	1.31	1.25
1	C	268	PHE	CE1-CZ	5.34	1.47	1.37
1	D	227	GLU	N-CA	5.31	1.56	1.46
1	A	95	GLU	CD-OE1	5.23	1.31	1.25
1	D	223	TRP	CZ2-CH2	5.17	1.47	1.37
1	C	211	ARG	CZ-NH2	5.17	1.39	1.33
1	B	253	GLN	C-O	5.15	1.33	1.23
1	B	227	GLU	CG-CD	5.05	1.59	1.51
1	A	282	ARG	CZ-NH1	5.04	1.39	1.33
1	A	242	GLN	CG-CD	5.01	1.62	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	TYR	CD1-CE1-CZ	-13.07	108.04	119.80
1	C	377	TRP	CG-CD1-NE1	-10.40	99.70	110.10
1	A	282	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	D	299	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	C	377	TRP	CD1-NE1-CE2	9.42	117.48	109.00
1	A	248	GLU	N-CA-CB	-9.38	93.71	110.60
1	A	299	ARG	NE-CZ-NH2	8.86	124.73	120.30
1	C	352	ARG	NE-CZ-NH2	8.85	124.73	120.30
1	C	243	ALA	CA-C-O	8.78	138.53	120.10
1	A	103	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	A	102	VAL	CB-CA-C	-7.68	96.81	111.40
1	B	254	VAL	N-CA-CB	7.54	128.08	111.50
1	D	282	ARG	CG-CD-NE	7.12	126.76	111.80
1	D	144	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	254	VAL	CG1-CB-CG2	-7.04	99.64	110.90
1	A	282	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	138	LEU	CB-CG-CD2	-6.78	99.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	B	257	PHE	CB-CG-CD1	6.77	125.54	120.80
1	B	254	VAL	CA-CB-CG1	6.74	121.01	110.90
1	A	289	LEU	CB-CG-CD1	-6.71	99.60	111.00
1	B	103	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	102	VAL	CB-CA-C	-6.50	99.04	111.40
1	C	377	TRP	CZ3-CH2-CZ2	-6.46	113.84	121.60
1	D	299	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	299	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	D	282	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	99	ASN	CB-CA-C	-6.29	97.82	110.40
1	A	316	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	144	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	334	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	D	194	LYS	CG-CD-CE	6.12	130.28	111.90
1	D	381	MET	N-CA-C	6.01	127.23	111.00
1	B	142	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	211	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	226	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	A	287	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	90	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	D	277	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	287	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	142	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	B	232	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	193	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	90	LEU	CA-CB-CG	-5.66	102.28	115.30
1	B	99	ASN	N-CA-CB	-5.53	100.64	110.60
1	D	267	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	334	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	211	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	377	TRP	NE1-CE2-CD2	-5.43	101.87	107.30
1	D	270	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	240	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	D	71	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	D	318	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	193	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	238	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	D	323	LYS	CD-CE-NZ	-5.33	99.45	111.70
1	D	286	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	C	103	ARG	CB-CG-CD	5.28	125.34	111.60
1	D	286	TYR	CE1-CZ-CE2	5.28	128.25	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	GLU	CB-CG-CD	-5.27	99.97	114.20
1	C	352	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	257	PHE	CB-CG-CD1	-5.15	117.20	120.80
1	D	269	ASP	O-C-N	-5.12	114.50	122.70
1	C	325	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	A	294	MET	CG-SD-CE	-5.06	92.10	100.20
1	B	265	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	148	SER	N-CA-CB	5.04	118.06	110.50
1	D	99	ASN	CB-CA-C	-5.02	100.36	110.40
1	B	218	HIS	CG-ND1-CE1	5.02	115.23	108.20
1	C	368	LEU	CB-CG-CD2	5.01	119.53	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	GLU	Peptide
1	A	347	GLY	Peptide
1	C	103	ARG	Peptide
1	C	253	GLN	Sidechain
1	D	144	ARG	Sidechain
1	D	187	GLU	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	2710	0	2699	57	0
1	B	2608	0	2605	84	0
1	C	2722	0	2714	74	0
1	D	2463	0	2470	89	0
2	A	43	0	30	4	0
2	B	43	0	30	8	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	17	0	0	0	0
3	D	17	0	0	0	0
4	A	15	0	9	0	0
4	B	15	0	9	0	0
4	D	15	0	9	0	0
5	A	13	0	5	0	0
All	All	10801	0	10640	279	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 13.

All (279) 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:GLU:CB	1:C:227:GLU:CG	1.79	1.60
1:C:232:ARG:CG	1:C:232:ARG:CB	1.89	1.50
1:C:243:ALA:CA	1:C:243:ALA:N	1.78	1.45
1:A:248:GLU:N	1:A:248:GLU:CA	1.84	1.38
1:B:262:GLU:O	1:B:266:SER:HB3	1.44	1.15
1:D:226:LEU:HB3	1:D:227:GLU:HA	1.31	1.13
1:D:224:GLY:HA2	1:D:225:LYS:HB2	1.30	1.10
1:B:269:ASP:HB3	1:B:272:ARG:NH2	1.70	1.05
1:C:154:GLN:HG3	1:D:42:TYR:HB2	1.46	0.98
1:B:293:LEU:HG	1:B:368:LEU:HD22	1.44	0.98
1:B:270:GLU:HB3	1:B:274:GLU:OE2	1.67	0.95
1:B:95:GLU:O	1:B:99:ASN:HB2	1.67	0.93
1:A:99:ASN:HB3	1:A:101:HIS:H	1.35	0.91
1:B:133:GLU:HB3	1:B:334:ARG:HH22	1.36	0.90
1:C:189:ASN:O	1:C:193:LEU:HB2	1.72	0.89
1:A:248:GLU:N	1:A:248:GLU:CB	2.37	0.86
1:D:382:ASN:HB2	1:D:383:PRO:HD2	1.54	0.86
1:D:226:LEU:CB	1:D:227:GLU:HA	2.07	0.84
1:C:173:VAL:HG11	1:C:353:SER:HB2	1.58	0.84
1:C:165:ILE:HG22	1:C:361:VAL:HG21	1.58	0.83
1:B:136:THR:HG21	1:D:299:ARG:NH2	1.92	0.83
1:D:352:ARG:O	1:D:355:VAL:HG12	1.80	0.82
1:C:325:ARG:O	1:C:329:VAL:HG13	1.82	0.80
1:D:226:LEU:HD21	1:D:377:TRP:CD2	2.17	0.79
1:B:261:LYS:HG2	1:B:265:LEU:HD21	1.65	0.79
1:D:165:ILE:HG22	1:D:361:VAL:HG21	1.65	0.78
1:B:72:PHE:HE1	2:B:401:HEM:HBB2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LEU:HB2	1:D:371:TYR:CE2	2.21	0.76
1:D:373:ILE:HD11	1:D:378:ILE:HG13	1.68	0.75
1:D:373:ILE:HD13	1:D:377:TRP:HB2	1.68	0.75
1:D:224:GLY:HA2	1:D:225:LYS:CB	2.15	0.75
1:A:136:THR:HG21	1:C:299:ARG:HH12	1.51	0.74
1:B:72:PHE:CE1	2:B:401:HEM:HBB2	2.22	0.74
1:B:266:SER:O	1:B:272:ARG:CZ	2.36	0.73
1:D:303:ARG:HD3	1:D:386:HIS:HA	1.71	0.73
1:C:251:GLU:HA	1:C:252:GLU:CB	2.18	0.73
1:A:293:LEU:HG	1:A:368:LEU:HD22	1.69	0.73
1:C:229:ASN:ND2	1:C:232:ARG:HH21	1.87	0.72
1:D:223:TRP:CE2	1:D:290:GLN:OE1	2.42	0.72
1:B:269:ASP:HB3	1:B:272:ARG:HH22	1.53	0.72
1:C:55:GLN:HG3	1:C:73:ILE:HD11	1.72	0.71
1:C:207:ALA:O	1:C:211:ARG:HD2	1.90	0.71
1:B:375:ARG:NH1	1:D:138:LEU:HD23	2.06	0.71
1:B:370:THR:HG22	1:D:337:GLY:HA3	1.71	0.70
1:D:57:LEU:H	1:D:57:LEU:HD22	1.55	0.70
1:A:346:SER:N	1:A:347:GLY:HA2	2.07	0.70
1:C:229:ASN:HD21	1:C:232:ARG:HH21	1.39	0.70
1:D:223:TRP:CZ2	1:D:290:GLN:OE1	2.45	0.70
1:A:328:HIS:HE1	2:A:401:HEM:C1A	2.10	0.70
1:B:259:LYS:HA	1:B:262:GLU:OE1	1.92	0.70
1:B:267:LEU:HD21	1:B:293:LEU:HD11	1.75	0.69
1:B:269:ASP:CB	1:B:272:ARG:NH2	2.53	0.69
1:C:243:ALA:N	1:C:243:ALA:C	2.41	0.67
1:B:258:GLN:O	1:B:262:GLU:OE1	2.11	0.67
1:B:266:SER:O	1:B:272:ARG:NH1	2.28	0.66
1:B:106:ARG:NH2	1:C:300:GLU:OE1	2.29	0.66
1:A:275:HIS:CE1	1:A:279:LYS:HD2	2.31	0.65
1:A:97:PHE:HA	1:A:102:VAL:CG2	2.26	0.65
1:C:171:MET:O	1:C:358:ARG:NH1	2.29	0.65
1:D:289:LEU:HD12	1:D:368:LEU:HD11	1.77	0.65
1:B:262:GLU:O	1:B:266:SER:CB	2.35	0.65
1:D:224:GLY:CA	1:D:225:LYS:HB2	2.17	0.65
1:D:96:ILE:HG22	1:D:102:VAL:HG22	1.78	0.65
1:A:97:PHE:HA	1:A:102:VAL:HG22	1.79	0.65
1:C:233:GLY:HA3	1:C:377:TRP:CE2	2.32	0.65
1:B:369:SER:O	1:B:372:LEU:HD22	1.97	0.65
1:C:90:LEU:HD11	1:C:201:LEU:HD22	1.78	0.64
1:D:162:GLU:O	1:D:167:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:O	1:A:99:ASN:HB2	1.97	0.64
1:D:382:ASN:HB2	1:D:383:PRO:CD	2.27	0.64
1:A:194:LYS:O	1:A:198:GLU:HG3	1.97	0.64
1:D:55:GLN:HG3	1:D:73:ILE:HD11	1.79	0.64
1:B:328:HIS:HE1	2:B:401:HEM:C1A	2.16	0.64
1:D:373:ILE:HD11	1:D:378:ILE:CG1	2.27	0.64
1:C:362:PHE:HB3	1:C:365:LEU:HD12	1.81	0.63
1:B:269:ASP:CB	1:B:272:ARG:HH22	2.11	0.63
1:B:133:GLU:HB3	1:B:334:ARG:NH2	2.11	0.63
1:B:136:THR:HG21	1:D:299:ARG:HH22	1.62	0.62
1:B:266:SER:HA	1:B:272:ARG:NH2	2.13	0.62
1:A:373:ILE:HD12	1:A:377:TRP:HB2	1.81	0.62
1:D:270:GLU:HB2	1:D:286:TYR:CE2	2.35	0.62
1:C:162:GLU:HB3	1:C:167:VAL:CG1	2.29	0.62
1:D:96:ILE:O	1:D:102:VAL:HG23	2.00	0.62
1:A:136:THR:HG22	1:A:138:LEU:H	1.66	0.61
1:D:190:GLU:O	1:D:194:LYS:HG3	2.01	0.60
1:A:70:HIS:HD2	1:B:85:GLN:OE1	1.83	0.60
1:B:60:GLU:HB2	1:B:65:LYS:HB2	1.82	0.60
1:A:309:GLN:HE22	1:D:309:GLN:HE22	1.50	0.59
1:C:97:PHE:HA	1:C:102:VAL:HG22	1.82	0.59
1:D:374:PRO:HD2	1:D:377:TRP:CE3	2.37	0.59
1:A:282:ARG:HH22	1:A:371:TYR:HE2	1.49	0.59
1:B:300:GLU:N	1:B:300:GLU:OE1	2.27	0.58
1:C:98:GLN:C	1:C:100:GLY:H	2.07	0.58
1:B:296:TYR:O	1:B:299:ARG:NH1	2.37	0.58
1:A:334:ARG:HB3	1:A:335:MET:HE3	1.85	0.58
1:D:99:ASN:HB3	1:D:101:HIS:H	1.67	0.58
1:D:109:LEU:O	1:D:113:SER:HB3	2.04	0.58
1:D:164:LYS:HD3	1:D:195:SER:HB2	1.85	0.58
1:B:271:LYS:HA	1:B:274:GLU:OE1	2.04	0.57
1:D:216:GLU:HB2	1:D:219:GLY:HA3	1.86	0.57
1:A:296:TYR:O	1:A:299:ARG:HD2	2.04	0.57
1:D:96:ILE:HG22	1:D:102:VAL:CG2	2.34	0.57
1:C:162:GLU:HB3	1:C:167:VAL:HG11	1.86	0.57
1:D:286:TYR:O	1:D:289:LEU:HB3	2.04	0.57
1:A:144:ARG:O	1:A:147:LEU:HB2	2.05	0.56
1:A:92:SER:OG	1:A:114:ARG:NH1	2.39	0.56
1:B:84:LYS:HG3	1:B:157:GLN:HE22	1.71	0.55
1:C:227:GLU:CA	1:C:227:GLU:CG	2.76	0.55
1:A:296:TYR:HE2	1:A:368:LEU:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:HIS:HB2	1:D:54:ALA:HB1	1.86	0.55
1:A:171:MET:HE1	1:A:358:ARG:HH11	1.72	0.55
1:C:375:ARG:HA	1:C:378:ILE:HD12	1.88	0.55
1:B:305:GLN:HG2	1:C:109:LEU:HG	1.89	0.55
1:C:242:GLN:C	1:C:243:ALA:CA	2.67	0.55
1:C:206:GLU:HB2	1:C:284:LEU:CD2	2.37	0.55
1:A:328:HIS:CE1	2:A:401:HEM:C1A	2.94	0.55
1:A:328:HIS:HE1	2:A:401:HEM:NA	2.03	0.55
1:C:333:HIS:HB2	1:C:348:TYR:CE1	2.42	0.55
1:B:375:ARG:HH11	1:D:138:LEU:HD23	1.72	0.54
1:D:162:GLU:HB3	1:D:167:VAL:HG11	1.88	0.54
1:D:71:LEU:HD11	1:D:131:ILE:HG22	1.89	0.54
1:B:328:HIS:CE1	2:B:401:HEM:C1A	2.95	0.54
1:B:362:PHE:HB3	1:B:365:LEU:HD12	1.90	0.54
1:D:325:ARG:O	1:D:329:VAL:HG23	2.07	0.54
1:A:169:GLN:OE1	1:A:196:GLU:HG2	2.08	0.53
1:D:373:ILE:CD1	1:D:377:TRP:HB2	2.37	0.53
1:B:109:LEU:HB2	1:C:305:GLN:HG2	1.89	0.53
1:A:136:THR:CG2	1:C:299:ARG:HH12	2.21	0.53
1:A:136:THR:HG21	1:C:299:ARG:NH1	2.23	0.53
1:A:380:LYS:H	1:A:380:LYS:CD	2.20	0.53
1:C:375:ARG:O	1:C:378:ILE:HD12	2.08	0.53
1:C:375:ARG:HA	1:C:378:ILE:CD1	2.38	0.53
1:B:348:TYR:HD1	1:B:349:HIS:HD2	1.57	0.53
1:B:259:LYS:HA	1:B:262:GLU:CD	2.29	0.53
1:D:303:ARG:NH1	1:D:385:ILE:O	2.39	0.53
1:D:187:GLU:C	1:D:189:ASN:N	2.61	0.52
1:A:128:GLN:HA	1:B:124:LEU:HD13	1.91	0.52
1:A:332:VAL:HG22	2:A:401:HEM:CHB	2.40	0.52
1:D:194:LYS:O	1:D:198:GLU:N	2.34	0.52
1:A:333:HIS:HB2	1:A:348:TYR:CE2	2.45	0.52
1:C:223:TRP:CE3	1:C:290:GLN:HG3	2.45	0.52
1:D:186:GLY:O	1:D:187:GLU:HB3	2.09	0.52
1:D:267:LEU:HB2	1:D:371:TYR:HE2	1.70	0.52
1:C:85:GLN:CD	1:D:71:LEU:HD22	2.30	0.52
1:C:229:ASN:HD21	1:C:232:ARG:NH2	2.05	0.52
1:D:187:GLU:C	1:D:189:ASN:H	2.13	0.52
1:B:136:THR:HG21	1:D:299:ARG:HH21	1.72	0.52
1:C:232:ARG:CG	1:C:232:ARG:CA	2.82	0.52
1:B:275:HIS:HE1	1:B:279:LYS:HE2	1.75	0.52
1:C:116:HIS:O	1:C:119:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ARG:HH11	1:C:276:LEU:HD11	1.75	0.52
1:A:142:ASP:CG	1:C:375:ARG:HE	2.14	0.51
1:C:175:TYR:O	1:C:176:ASN:HB2	2.10	0.51
1:B:193:LEU:O	1:B:197:GLN:HG2	2.11	0.51
1:B:275:HIS:CE1	1:B:279:LYS:HE2	2.45	0.51
1:C:144:ARG:NH2	1:C:336:LEU:HD22	2.26	0.51
1:B:162:GLU:HB3	1:B:167:VAL:HG22	1.93	0.51
1:A:138:LEU:HD12	1:C:372:LEU:HD11	1.92	0.51
1:A:171:MET:CE	1:A:358:ARG:HH11	2.24	0.50
1:D:167:VAL:HA	1:D:361:VAL:HG22	1.93	0.50
1:C:159:ARG:HH11	1:C:172:ARG:HH12	1.58	0.50
1:D:160:LEU:O	1:D:164:LYS:HG2	2.12	0.50
1:D:98:GLN:HG3	1:D:204:LEU:HD21	1.94	0.50
1:D:59:SER:HB3	1:D:66:ILE:H	1.77	0.50
1:A:65:LYS:H	1:A:65:LYS:NZ	2.09	0.50
1:C:227:GLU:CB	1:C:227:GLU:CD	2.73	0.50
1:A:226:LEU:HG	1:A:230:ILE:HD12	1.94	0.50
1:D:313:SER:O	1:D:316:ASP:HB2	2.13	0.49
1:B:293:LEU:HG	1:B:368:LEU:CD2	2.31	0.48
1:C:284:LEU:N	1:C:364:ASP:OD2	2.41	0.48
1:B:327:ASN:N	1:B:327:ASN:HD22	2.10	0.48
1:C:115:MET:HE2	1:C:201:LEU:HD21	1.95	0.48
1:D:95:GLU:O	1:D:99:ASN:HB2	2.14	0.48
1:B:270:GLU:HG2	1:B:286:TYR:CD2	2.48	0.48
1:B:226:LEU:HG	1:B:230:ILE:HD12	1.96	0.48
1:C:351:LEU:HD21	2:C:401:HEM:HAA2	1.95	0.48
1:B:385:ILE:HG22	1:B:386:HIS:HD2	1.78	0.48
1:B:157:GLN:HA	1:B:160:LEU:HD12	1.95	0.48
1:B:190:GLU:O	1:B:194:LYS:HB2	2.15	0.47
1:B:269:ASP:HB3	1:B:272:ARG:CZ	2.40	0.47
1:B:303:ARG:H	1:B:386:HIS:CE1	2.33	0.47
1:B:159:ARG:NH1	2:B:401:HEM:O2D	2.28	0.47
1:C:189:ASN:O	1:C:193:LEU:N	2.45	0.47
1:D:382:ASN:CB	1:D:383:PRO:HD2	2.36	0.47
1:A:358:ARG:HD3	1:A:358:ARG:HA	1.62	0.47
1:B:232:ARG:HH11	1:B:232:ARG:HB2	1.80	0.47
1:D:151:SER:HB3	1:D:154:GLN:HG3	1.97	0.46
1:D:85:GLN:NE2	1:D:89:GLU:OE2	2.49	0.46
1:B:299:ARG:HH11	1:B:299:ARG:HB3	1.81	0.46
1:C:234:LEU:HD13	1:C:261:LYS:HG3	1.97	0.46
1:D:331:MET:CE	1:D:331:MET:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLN:HG2	1:D:84:LYS:HE2	1.97	0.46
1:B:136:THR:HG22	1:B:138:LEU:H	1.80	0.46
1:B:334:ARG:CG	1:B:334:ARG:HH11	2.29	0.45
1:D:328:HIS:O	1:D:332:VAL:HG23	2.15	0.45
1:A:123:LYS:HE2	1:A:123:LYS:HB3	1.59	0.45
1:C:185:LYS:HB2	1:C:189:ASN:HD22	1.81	0.45
1:B:99:ASN:HB3	1:B:101:HIS:H	1.80	0.45
1:D:73:ILE:O	1:D:77:GLN:HG3	2.16	0.45
1:C:46:LEU:HB2	1:C:48:LEU:HG	1.97	0.45
1:B:303:ARG:HB2	1:B:386:HIS:CE1	2.51	0.45
1:C:154:GLN:HG3	1:D:42:TYR:CB	2.32	0.45
1:B:96:ILE:HG22	1:B:102:VAL:HG13	1.99	0.45
1:B:210:GLU:HG2	1:B:287:ARG:HB3	1.98	0.45
1:B:129:PHE:O	1:B:133:GLU:HG3	2.17	0.44
1:B:152:GLY:HA3	2:B:401:HEM:C4D	2.52	0.44
1:B:69:GLU:HG3	1:B:143:PHE:CD2	2.52	0.44
1:C:175:TYR:CE1	1:C:347:GLY:HA2	2.52	0.44
1:D:357:ASP:HA	1:D:360:LYS:HG3	1.98	0.44
1:B:303:ARG:H	1:B:386:HIS:HE1	1.64	0.44
1:D:226:LEU:HD21	1:D:377:TRP:CG	2.52	0.44
1:A:79:TYR:CD1	1:A:125:LEU:HD22	2.53	0.44
1:A:241:ILE:O	1:A:242:GLN:OE1	2.35	0.44
1:D:296:TYR:O	1:D:299:ARG:NH1	2.39	0.44
1:D:335:MET:HG3	2:D:401:HEM:CBB	2.48	0.44
1:A:223:TRP:CZ3	1:A:290:GLN:HG2	2.53	0.44
1:B:269:ASP:H	1:B:272:ARG:HH22	1.65	0.44
1:D:309:GLN:O	1:D:313:SER:HB2	2.17	0.44
1:B:353:SER:O	1:B:356:SER:HB2	2.18	0.44
1:C:301:GLU:O	1:C:302:PRO:C	2.56	0.44
1:C:84:LYS:HE3	1:D:55:GLN:OE1	2.17	0.44
1:A:269:ASP:CG	1:A:272:ARG:HB2	2.38	0.44
1:C:329:VAL:CG1	1:C:351:LEU:HB3	2.48	0.44
1:D:373:ILE:HD13	1:D:377:TRP:CB	2.45	0.44
1:C:333:HIS:HB2	1:C:348:TYR:HE1	1.83	0.43
1:A:248:GLU:C	1:A:248:GLU:N	2.66	0.43
1:D:226:LEU:HD12	1:D:226:LEU:HA	1.70	0.43
1:A:132:LEU:HD23	1:A:331:MET:SD	2.58	0.43
1:B:334:ARG:HG2	1:B:334:ARG:HH11	1.83	0.43
1:D:329:VAL:HG22	1:D:351:LEU:HB3	2.00	0.43
1:A:346:SER:H	1:A:347:GLY:HA2	1.78	0.43
1:C:241:ILE:C	1:C:243:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TRP:CE3	1:A:290:GLN:HG2	2.53	0.43
1:B:269:ASP:O	1:B:270:GLU:C	2.57	0.43
1:D:96:ILE:C	1:D:102:VAL:HG23	2.38	0.43
1:A:380:LYS:H	1:A:380:LYS:HD2	1.82	0.43
1:B:354:THR:HG22	1:B:359:TYR:CZ	2.54	0.43
1:D:223:TRP:CZ2	1:D:286:TYR:CE2	3.06	0.43
1:D:296:TYR:HE2	1:D:369:SER:HG	1.64	0.43
1:B:261:LYS:HG2	1:B:265:LEU:CD2	2.43	0.43
1:A:267:LEU:HD13	1:A:371:TYR:CG	2.54	0.43
1:C:144:ARG:O	1:C:147:LEU:HB2	2.18	0.43
1:C:241:ILE:C	1:C:243:ALA:N	2.73	0.42
1:D:326:TYR:HB2	1:D:355:VAL:HG21	2.00	0.42
1:D:269:ASP:CG	1:D:272:ARG:HB2	2.39	0.42
1:A:95:GLU:OE1	1:A:98:GLN:HG3	2.20	0.42
1:C:162:GLU:HB3	1:C:167:VAL:HG12	1.97	0.42
1:C:81:LEU:HD12	1:D:81:LEU:HD12	2.01	0.42
1:D:136:THR:HA	1:D:334:ARG:HH22	1.83	0.42
1:A:327:ASN:HD22	1:A:327:ASN:N	2.17	0.42
1:D:57:LEU:H	1:D:57:LEU:CD2	2.29	0.42
1:B:199:LYS:HD3	1:B:204:LEU:HD21	2.02	0.42
2:B:401:HEM:HHD	2:B:401:HEM:CBC	2.50	0.42
1:C:241:ILE:O	1:C:243:ALA:N	2.53	0.42
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.49	0.42
1:B:162:GLU:HB3	1:B:167:VAL:CG2	2.50	0.42
1:C:233:GLY:HA3	1:C:377:TRP:CZ2	2.54	0.42
1:B:262:GLU:OE2	1:B:263:VAL:HG23	2.20	0.41
1:A:271:LYS:H	1:A:271:LYS:HG2	1.33	0.41
1:A:209:LEU:HD21	1:A:311:LEU:HD21	2.02	0.41
1:B:306:VAL:HG21	1:C:305:GLN:HE21	1.84	0.41
1:C:46:LEU:O	1:D:77:GLN:NE2	2.45	0.41
1:D:269:ASP:OD2	1:D:272:ARG:HB2	2.20	0.41
1:D:48:LEU:HA	1:D:48:LEU:HD23	1.93	0.41
1:A:275:HIS:HE1	1:A:279:LYS:HD2	1.82	0.41
1:B:332:VAL:HG22	2:B:401:HEM:CHB	2.50	0.41
1:C:232:ARG:O	1:C:236:GLU:HB2	2.21	0.41
1:B:259:LYS:CA	1:B:262:GLU:OE1	2.66	0.41
1:D:267:LEU:HD22	1:D:371:TYR:CD2	2.55	0.41
1:A:171:MET:HE1	1:A:358:ARG:NH1	2.35	0.41
1:D:200:THR:C	1:D:204:LEU:HD12	2.41	0.41
1:A:115:MET:HE3	1:A:317:ILE:HD12	2.03	0.41
1:B:266:SER:CA	1:B:272:ARG:NH2	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LYS:O	1:B:363:VAL:HG12	2.21	0.40
1:B:165:ILE:HG22	1:B:361:VAL:HG21	2.04	0.40
1:C:154:GLN:HG2	1:C:154:GLN:H	1.76	0.40
1:B:262:GLU:N	1:B:262:GLU:CD	2.75	0.40
1:C:328:HIS:CE1	2:C:401:HEM:C1A	3.09	0.40
1:D:152:GLY:HA3	2:D:401:HEM:C4D	2.57	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	314/391 (80%)	296 (94%)	15 (5%)	3 (1%)	15	23
1	B	301/391 (77%)	270 (90%)	24 (8%)	7 (2%)	6	8
1	C	315/391 (81%)	280 (89%)	32 (10%)	3 (1%)	15	23
1	D	283/391 (72%)	247 (87%)	26 (9%)	10 (4%)	3	4
All	All	1213/1564 (78%)	1093 (90%)	97 (8%)	23 (2%)	8	11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	241	ILE
1	B	384	THR
1	C	176	ASN
1	D	223	TRP
1	D	225	LYS
1	B	106	ARG
1	B	270	GLU
1	C	195	SER

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Mol	Chain	Res	Type
1	C	242	GLN
1	D	62	LYS
1	D	187	GLU
1	D	358	ARG
1	D	382	ASN
1	B	188	GLU
1	B	368	LEU
1	B	383	PRO
1	D	188	GLU
1	B	233	GLY
1	D	99	ASN
1	D	226	LEU
1	D	385	ILE
1	A	347	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	297/356 (83%)	260 (88%)	37 (12%)	4	6
1	B	287/356 (81%)	244 (85%)	43 (15%)	3	3
1	C	297/356 (83%)	250 (84%)	47 (16%)	2	2
1	D	272/356 (76%)	223 (82%)	49 (18%)	1	1
All	All	1153/1424 (81%)	977 (85%)	176 (15%)	3	3

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	65	LYS
1	A	90	LEU
1	A	99	ASN
1	A	102	VAL
1	A	110	LYS
1	A	138	LEU

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	147	LEU
1	A	148	SER
1	A	159	ARG
1	A	168	LEU
1	A	171	MET
1	A	187	GLU
1	A	191	LEU
1	A	193	LEU
1	A	196	GLU
1	A	225	LYS
1	A	236	GLU
1	A	242	GLN
1	A	251	GLU
1	A	289	LEU
1	A	299	ARG
1	A	300	GLU
1	A	303	ARG
1	A	318	ASP
1	A	323	LYS
1	A	327	ASN
1	A	329	VAL
1	A	331	MET
1	A	338	SER
1	A	345	SER
1	A	352	ARG
1	A	353	SER
1	A	358	ARG
1	A	380	LYS
1	A	381	MET
1	B	50	LYS
1	B	62	LYS
1	B	90	LEU
1	B	115	MET
1	B	119	SER
1	B	124	LEU
1	B	138	LEU
1	B	144	ARG
1	B	159	ARG
1	B	168	LEU
1	B	191	LEU
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	194	LYS
1	B	197	GLN
1	B	225	LYS
1	B	228	LYS
1	B	231	THR
1	B	232	ARG
1	B	237	GLU
1	B	253	GLN
1	B	257	PHE
1	B	259	LYS
1	B	262	GLU
1	B	263	VAL
1	B	265	LEU
1	B	271	LYS
1	B	272	ARG
1	B	274	GLU
1	B	278	SER
1	B	296	TYR
1	B	299	ARG
1	B	300	GLU
1	B	303	ARG
1	B	318	ASP
1	B	331	MET
1	B	334	ARG
1	B	352	ARG
1	B	356	SER
1	B	363	VAL
1	B	370	THR
1	B	372	LEU
1	B	375	ARG
1	B	382	ASN
1	C	41	ILE
1	C	44	ASN
1	C	73	ILE
1	C	92	SER
1	C	95	GLU
1	C	98	GLN
1	C	99	ASN
1	C	102	VAL
1	C	109	LEU
1	C	123	LYS
1	C	138	LEU

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Mol	Chain	Res	Type
1	C	144	ARG
1	C	147	LEU
1	C	154	GLN
1	C	159	ARG
1	C	169	GLN
1	C	176	ASN
1	C	177	ARG
1	C	187	GLU
1	C	192	LEU
1	C	193	LEU
1	C	195	SER
1	C	199	LYS
1	C	218	HIS
1	C	225	LYS
1	C	228	LYS
1	C	229	ASN
1	C	236	GLU
1	C	240	ARG
1	C	256	GLU
1	C	259	LYS
1	C	272	ARG
1	C	279	LYS
1	C	282	ARG
1	C	293	LEU
1	C	296	TYR
1	C	299	ARG
1	C	317	ILE
1	C	319	SER
1	C	323	LYS
1	C	329	VAL
1	C	349	HIS
1	C	353	SER
1	C	358	ARG
1	C	372	LEU
1	C	373	ILE
1	C	375	ARG
1	D	41	ILE
1	D	57	LEU
1	D	61	THR
1	D	62	LYS
1	D	66	ILE
1	D	71	LEU

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Mol	Chain	Res	Type
1	D	73	ILE
1	D	95	GLU
1	D	99	ASN
1	D	110	LYS
1	D	113	SER
1	D	119	SER
1	D	127	GLN
1	D	136	THR
1	D	138	LEU
1	D	141	ASN
1	D	164	LYS
1	D	185	LYS
1	D	187	GLU
1	D	188	GLU
1	D	192	LEU
1	D	195	SER
1	D	210	GLU
1	D	221	ASN
1	D	223	TRP
1	D	225	LYS
1	D	226	LEU
1	D	227	GLU
1	D	264	LEU
1	D	266	SER
1	D	271	LYS
1	D	272	ARG
1	D	276	LEU
1	D	277	LEU
1	D	279	LYS
1	D	287	ARG
1	D	290	GLN
1	D	293	LEU
1	D	297	PHE
1	D	299	ARG
1	D	313	SER
1	D	331	MET
1	D	352	ARG
1	D	363	VAL
1	D	369	SER
1	D	376	HIS
1	D	380	LYS
1	D	382	ASN

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Mol	Chain	Res	Type
1	D	385	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	99	ASN
1	A	128	GLN
1	A	242	GLN
1	A	275	HIS
1	A	305	GLN
1	A	309	GLN
1	A	327	ASN
1	A	349	HIS
1	A	367	ASN
1	B	44	ASN
1	B	98	GLN
1	B	141	ASN
1	B	157	GLN
1	B	197	GLN
1	B	275	HIS
1	B	327	ASN
1	B	349	HIS
1	B	382	ASN
1	B	386	HIS
1	C	64	ASN
1	C	141	ASN
1	C	189	ASN
1	C	197	GLN
1	C	229	ASN
1	C	275	HIS
1	C	290	GLN
1	C	305	GLN
1	C	333	HIS
1	C	349	HIS
1	D	70	HIS
1	D	99	ASN
1	D	163	ASN
1	D	273	HIS
1	D	382	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	401	1,3	27,50,50	1.14	1 (3%)	17,82,82	2.84	7 (41%)
2	HEM	D	401	1,3	27,50,50	0.96	1 (3%)	17,82,82	2.41	7 (41%)
5	CIT	A	404	-	3,12,12	0.85	0	3,17,17	2.90	1 (33%)
3	9R9	C	402	2	18,19,19	2.79	8 (44%)	19,28,28	1.88	4 (21%)
2	HEM	B	401	1,3	27,50,50	1.13	2 (7%)	17,82,82	2.93	7 (41%)
2	HEM	C	401	1,3	27,50,50	1.02	2 (7%)	17,82,82	2.05	5 (29%)
3	9R9	A	402	2	18,19,19	2.44	7 (38%)	19,28,28	1.34	3 (15%)
4	TRP	D	403	-	12,16,16	2.12	3 (25%)	12,22,22	1.12	1 (8%)
4	TRP	B	403	-	12,16,16	1.99	5 (41%)	12,22,22	1.07	1 (8%)
3	9R9	D	402	2	18,19,19	2.35	7 (38%)	19,28,28	3.88	8 (42%)
3	9R9	B	402	2	18,19,19	3.16	7 (38%)	19,28,28	1.78	5 (26%)
4	TRP	A	403	-	12,16,16	2.24	4 (33%)	12,22,22	1.34	1 (8%)

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	401	1,3	-	2/6/54/54	-
2	HEM	D	401	1,3	-	1/6/54/54	-
5	CIT	A	404	-	-	5/6/16/16	-
3	9R9	C	402	2	-	0/6/16/16	0/3/3/3
2	HEM	B	401	1,3	-	0/6/54/54	-
2	HEM	C	401	1,3	-	0/6/54/54	-
3	9R9	A	402	2	-	0/6/16/16	0/3/3/3
4	TRP	D	403	-	-	0/3/8/8	0/2/2/2
4	TRP	B	403	-	-	0/3/8/8	0/2/2/2
3	9R9	D	402	2	-	0/6/16/16	0/3/3/3
3	9R9	B	402	2	-	0/6/16/16	0/3/3/3
4	TRP	A	403	-	-	1/3/8/8	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	9R9	CAJ-CAF	-8.80	1.43	1.53
3	C	402	9R9	CAJ-CAF	-6.62	1.45	1.53
3	B	402	9R9	CAC-CAD	-5.89	1.32	1.41
3	A	402	9R9	CAC-CAD	-5.61	1.33	1.41
3	C	402	9R9	CAC-CAD	-5.41	1.33	1.41
3	A	402	9R9	CAJ-CAF	-5.22	1.47	1.53
3	D	402	9R9	CAC-CAD	-4.90	1.34	1.41
3	D	402	9R9	CAB-CLA	-4.86	1.63	1.74
3	B	402	9R9	CAB-CLA	-4.72	1.64	1.74
4	D	403	TRP	CZ2-CE2	-4.66	1.33	1.41
3	C	402	9R9	CAK-CAJ	4.49	1.59	1.53
4	A	403	TRP	CZ2-CE2	-4.38	1.34	1.41
3	A	402	9R9	CAB-CLA	-4.17	1.65	1.74
3	D	402	9R9	CAK-CAJ	-4.00	1.48	1.53
2	A	401	HEM	C4D-C3D	4.00	1.51	1.42
4	A	403	TRP	CE3-CD2	-3.94	1.34	1.42
4	D	403	TRP	CE3-CD2	-3.65	1.34	1.42
3	B	402	9R9	CAF-CAE	-3.44	1.36	1.43
2	B	401	HEM	C4D-C3D	3.24	1.49	1.42
4	B	403	TRP	CE3-CD2	-3.20	1.35	1.42
4	B	403	TRP	CZ2-CE2	-3.09	1.36	1.41
3	B	402	9R9	CAI-CAE	-3.05	1.34	1.40
4	A	403	TRP	CD2-CE2	-3.00	1.34	1.42
3	C	402	9R9	CAF-CAE	-2.76	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	9R9	CAI-CAE	-2.67	1.35	1.40
4	D	403	TRP	CD2-CE2	-2.65	1.35	1.42
4	B	403	TRP	CB-CG	2.62	1.58	1.51
3	C	402	9R9	CAE-CAD	-2.61	1.35	1.42
4	B	403	TRP	CD2-CE2	-2.58	1.35	1.42
3	D	402	9R9	CAI-CAE	-2.53	1.35	1.40
2	C	401	HEM	C1C-C2C	-2.49	1.36	1.42
2	C	401	HEM	C4D-C3D	2.47	1.48	1.42
3	B	402	9R9	CAK-CAJ	2.47	1.56	1.53
3	C	402	9R9	CAB-CLA	-2.41	1.69	1.74
4	B	403	TRP	CZ3-CE3	2.32	1.42	1.36
2	D	401	HEM	C4D-C3D	2.26	1.47	1.42
3	D	402	9R9	NAH-NAG	-2.23	1.33	1.37
3	A	402	9R9	CAF-CAE	-2.21	1.39	1.43
2	B	401	HEM	C3B-C2B	-2.18	1.37	1.40
3	A	402	9R9	CAC-CAB	2.15	1.40	1.36
3	A	402	9R9	CAE-CAD	-2.08	1.37	1.42
3	B	402	9R9	CAE-CAD	-2.08	1.37	1.42
3	A	402	9R9	CAI-CAE	-2.06	1.36	1.40
3	C	402	9R9	CAK-CAL	2.04	1.57	1.52
3	D	402	9R9	CAJ-CAF	-2.02	1.51	1.53
3	D	402	9R9	CAE-CAD	-2.02	1.37	1.42
4	A	403	TRP	CD1-NE1	-2.01	1.32	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	9R9	OAP-CAJ-CAF	-10.82	91.41	109.99
3	D	402	9R9	CAO-CAJ-CAK	6.91	118.18	108.80
2	B	401	HEM	CBD-CAD-C3D	-6.87	99.81	112.48
2	B	401	HEM	CAD-CBD-CGD	6.54	123.64	112.67
2	A	401	HEM	CAD-CBD-CGD	6.35	123.33	112.67
3	C	402	9R9	CAL-CAK-CAJ	6.14	116.02	112.60
2	C	401	HEM	CBD-CAD-C3D	-6.09	101.26	112.48
2	A	401	HEM	CBD-CAD-C3D	-5.95	101.51	112.48
3	D	402	9R9	OAP-CAJ-CAK	5.87	121.00	107.69
3	B	402	9R9	CAL-CAK-CAJ	5.10	115.44	112.60
2	A	401	HEM	C1D-C2D-C3D	-4.93	103.57	107.00
3	D	402	9R9	CAL-CAK-CAJ	-4.85	109.89	112.60
2	B	401	HEM	C1D-C2D-C3D	-4.85	103.62	107.00
3	D	402	9R9	CAA-CAF-CAE	-4.83	114.77	119.98
2	D	401	HEM	CAD-CBD-CGD	4.71	120.58	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	CIT	C3-C4-C5	4.59	122.33	114.98
3	D	402	9R9	OAP-CAJ-CAO	4.37	117.60	107.69
2	D	401	HEM	CMD-C2D-C1D	-4.03	122.27	128.46
2	D	401	HEM	CMD-C2D-C3D	3.75	132.02	124.94
2	D	401	HEM	CMB-C2B-C3B	3.56	131.33	124.68
4	A	403	TRP	CB-CG-CD1	-3.43	123.73	127.97
3	C	402	9R9	CAO-CAJ-CAK	3.07	112.97	108.80
3	B	402	9R9	CAA-CAF-CAE	-3.00	116.74	119.98
2	C	401	HEM	CMA-C3A-C4A	-2.85	124.08	128.46
2	D	401	HEM	CBA-CAA-C2A	2.85	117.75	112.49
2	D	401	HEM	CMA-C3A-C4A	-2.77	124.21	128.46
3	D	402	9R9	CAN-CAO-CAJ	-2.66	111.12	112.60
3	A	402	9R9	CAC-CAB-CLA	-2.64	116.34	119.64
3	D	402	9R9	CAB-CAA-CAF	2.62	122.00	118.39
2	A	401	HEM	C4A-C3A-C2A	-2.58	105.20	107.00
3	A	402	9R9	CAA-CAF-CAE	-2.57	117.20	119.98
3	A	402	9R9	CAO-CAJ-CAK	2.53	112.24	108.80
2	A	401	HEM	CMB-C2B-C3B	2.52	129.38	124.68
4	D	403	TRP	CE3-CD2-CE2	2.50	121.49	118.17
2	B	401	HEM	CMB-C2B-C3B	2.36	129.09	124.68
2	A	401	HEM	CBA-CAA-C2A	-2.35	108.14	112.49
2	C	401	HEM	CMC-C2C-C3C	2.34	129.06	124.68
2	B	401	HEM	CAA-CBA-CGA	2.30	116.53	112.67
2	C	401	HEM	CMB-C2B-C3B	2.29	128.97	124.68
2	D	401	HEM	C3B-C4B-NB	-2.28	106.26	109.21
2	B	401	HEM	CMA-C3A-C4A	-2.26	124.98	128.46
4	B	403	TRP	CB-CG-CD1	-2.21	125.24	127.97
3	B	402	9R9	CAB-CAC-CAD	-2.17	117.66	119.50
3	B	402	9R9	CAN-CAO-CAJ	-2.14	111.40	112.60
2	B	401	HEM	C3B-C4B-NB	-2.10	106.50	109.21
2	A	401	HEM	CMA-C3A-C2A	2.09	128.88	124.94
2	C	401	HEM	CMA-C3A-C2A	2.08	128.85	124.94
3	C	402	9R9	CAA-CAF-CAE	-2.06	117.75	119.98
3	C	402	9R9	OAP-CAJ-CAK	-2.05	103.04	107.69
3	B	402	9R9	CAO-CAJ-CAK	2.03	111.56	108.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	HEM	C3D-CAD-CBD-CGD
5	A	404	CIT	C2-C3-C4-C5

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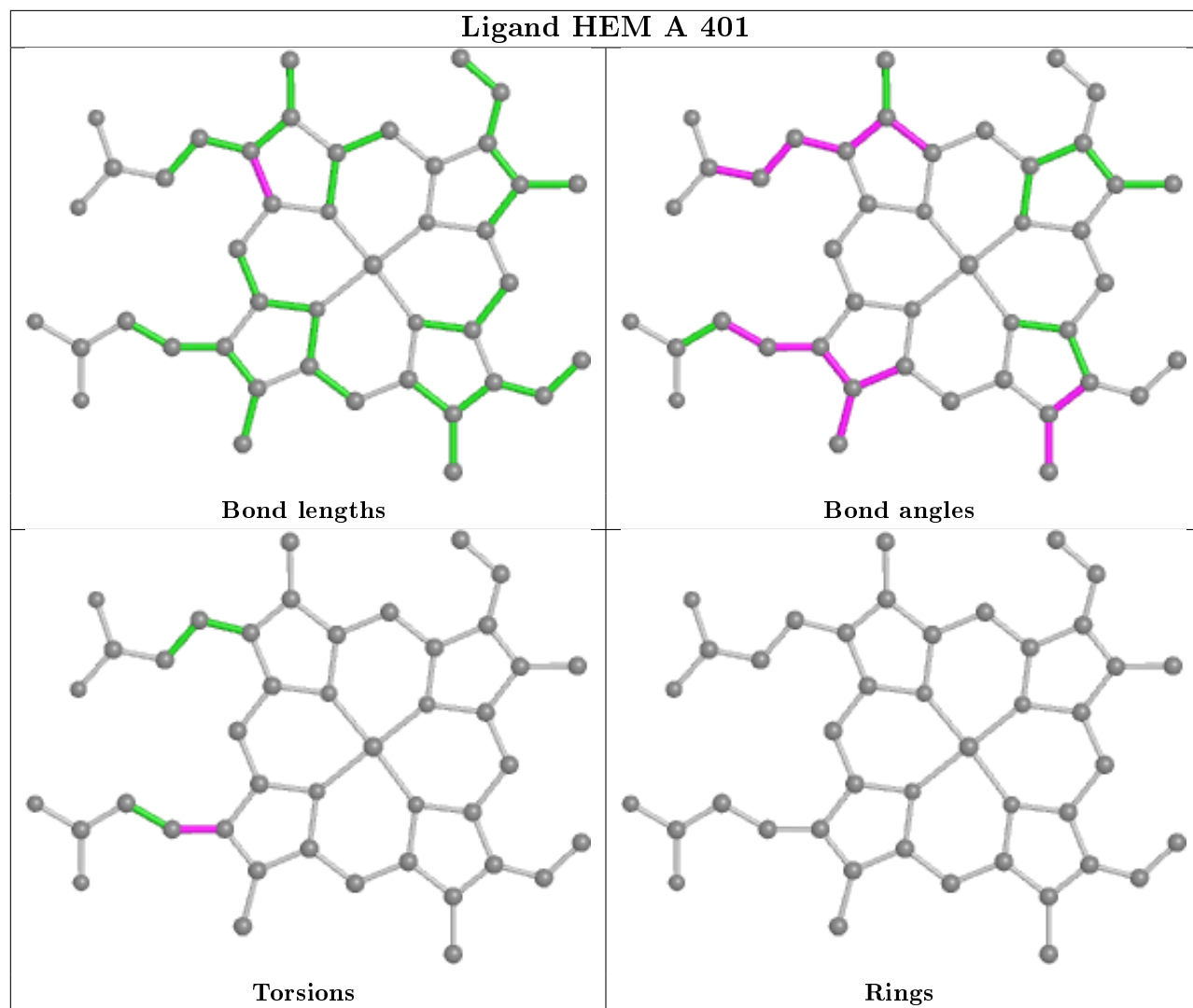
Mol	Chain	Res	Type	Atoms
5	A	404	CIT	C6-C3-C4-C5
5	A	404	CIT	C1-C2-C3-C4
5	A	404	CIT	O7-C3-C4-C5
5	A	404	CIT	C1-C2-C3-C6
2	A	401	HEM	C1A-C2A-CAA-CBA
2	A	401	HEM	C3A-C2A-CAA-CBA
4	A	403	TRP	CA-CB-CG-CD1

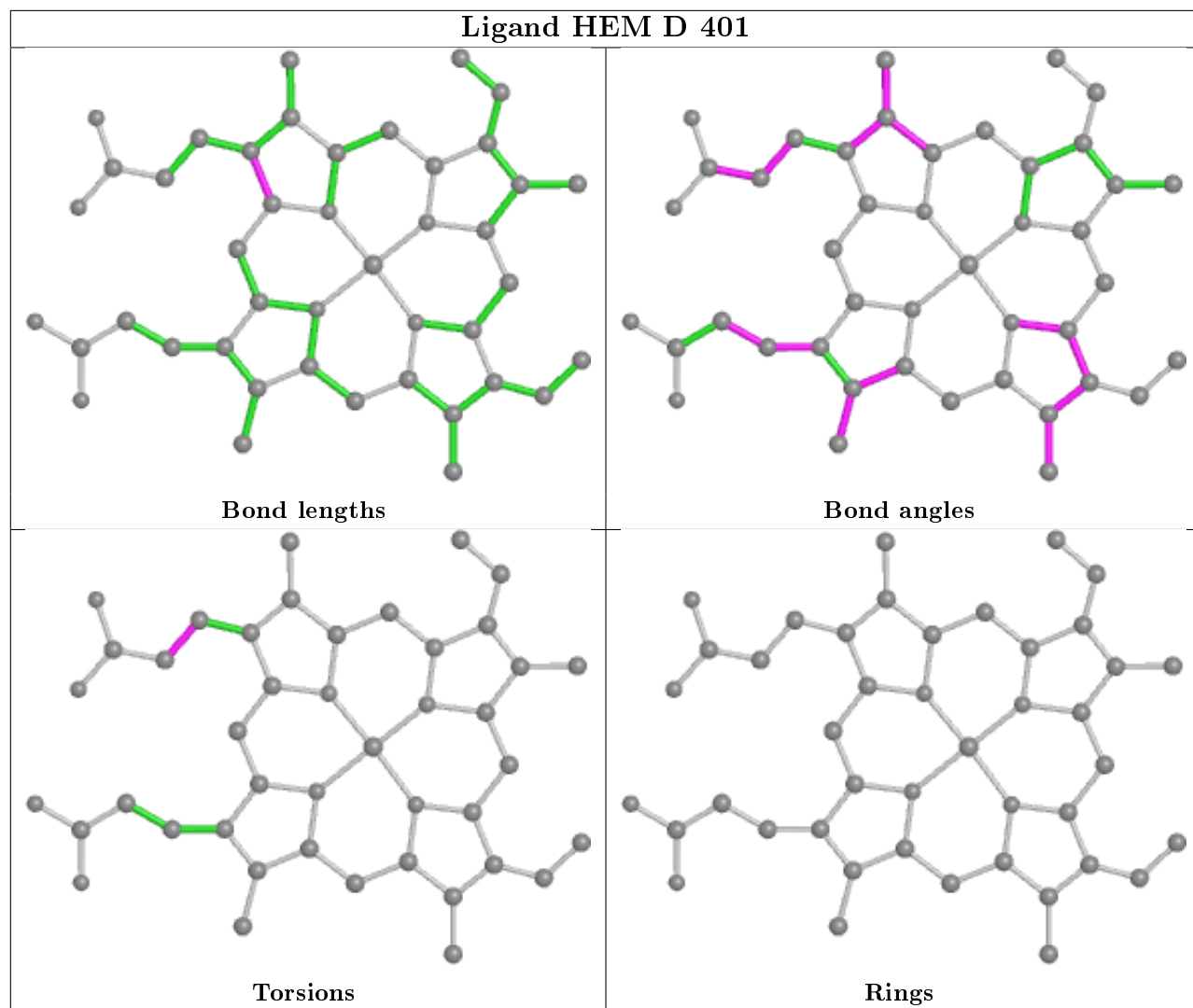
There are no ring outliers.

4 monomers are involved in 16 short contacts:

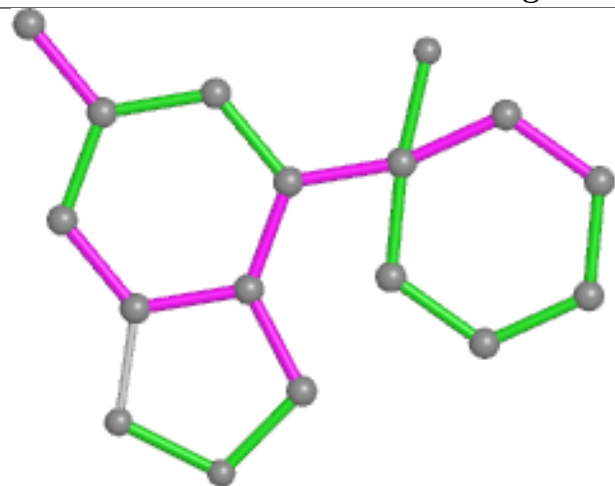
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	4	0
2	D	401	HEM	2	0
2	B	401	HEM	8	0
2	C	401	HEM	2	0

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

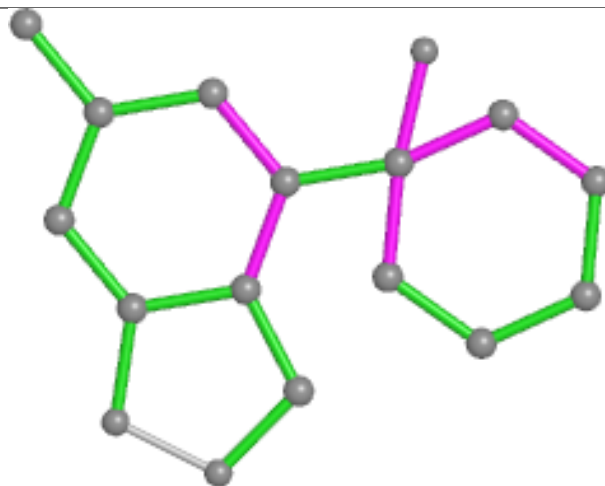




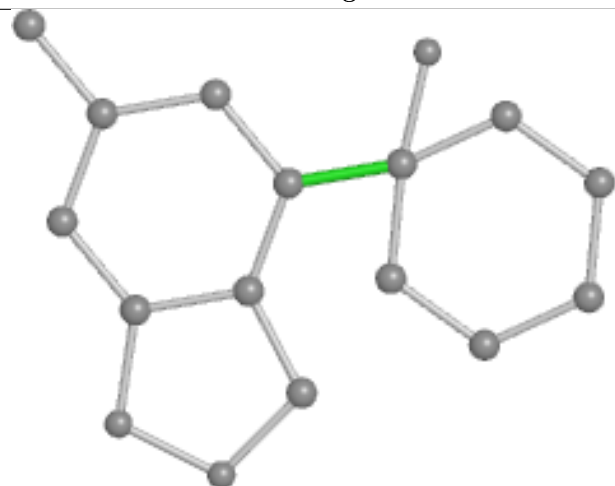
Ligand 9R9 C 402



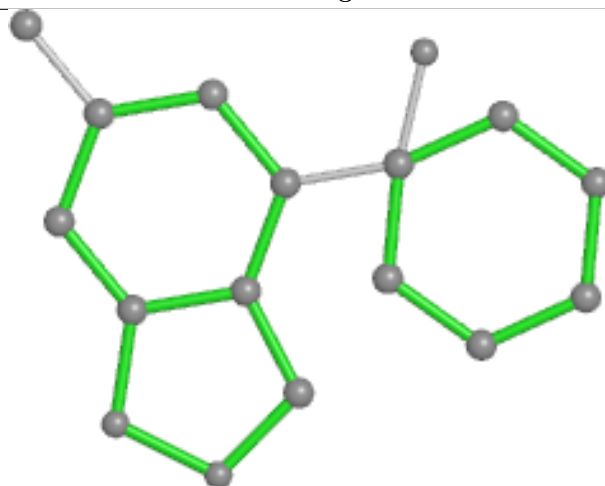
Bond lengths



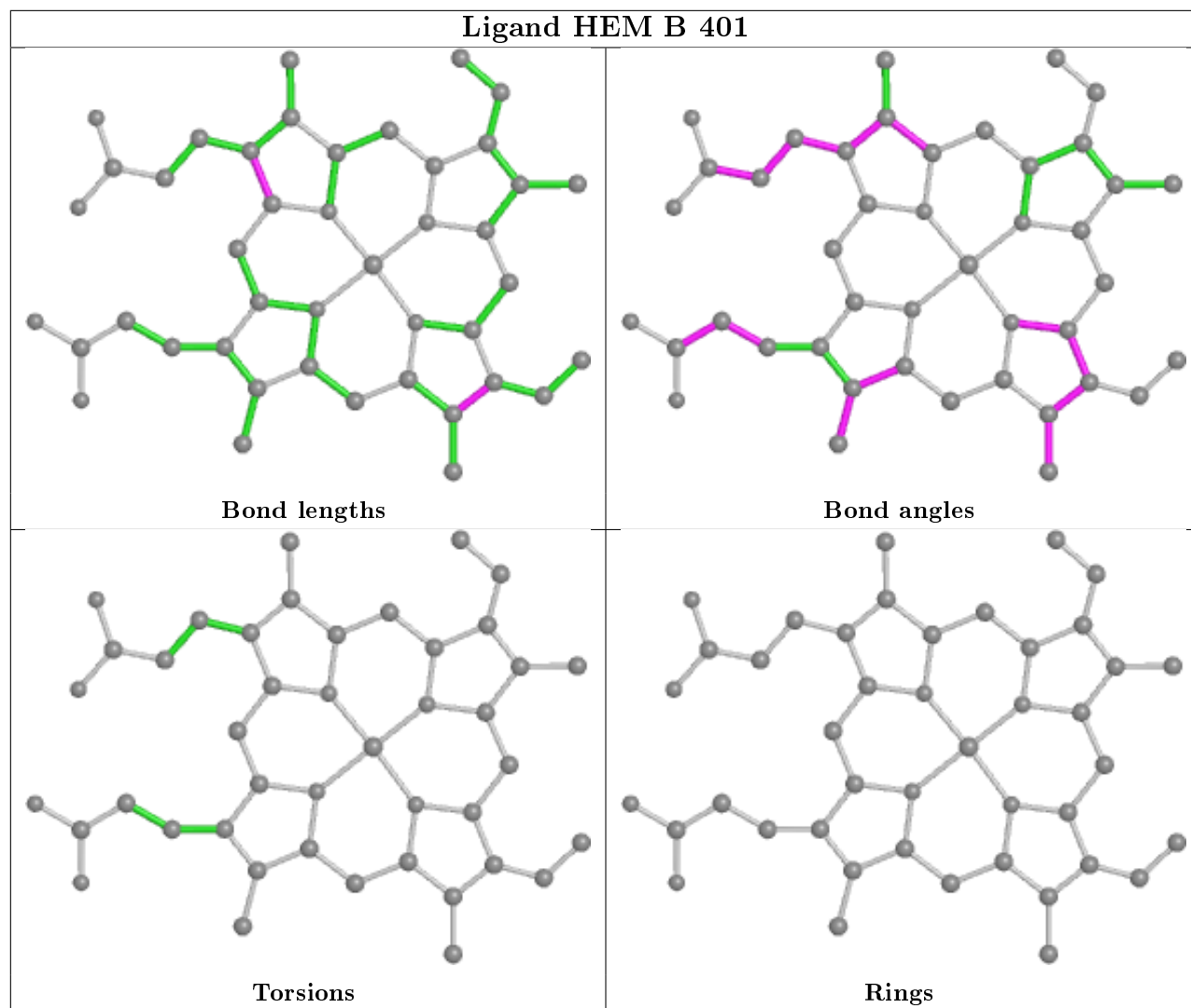
Bond angles

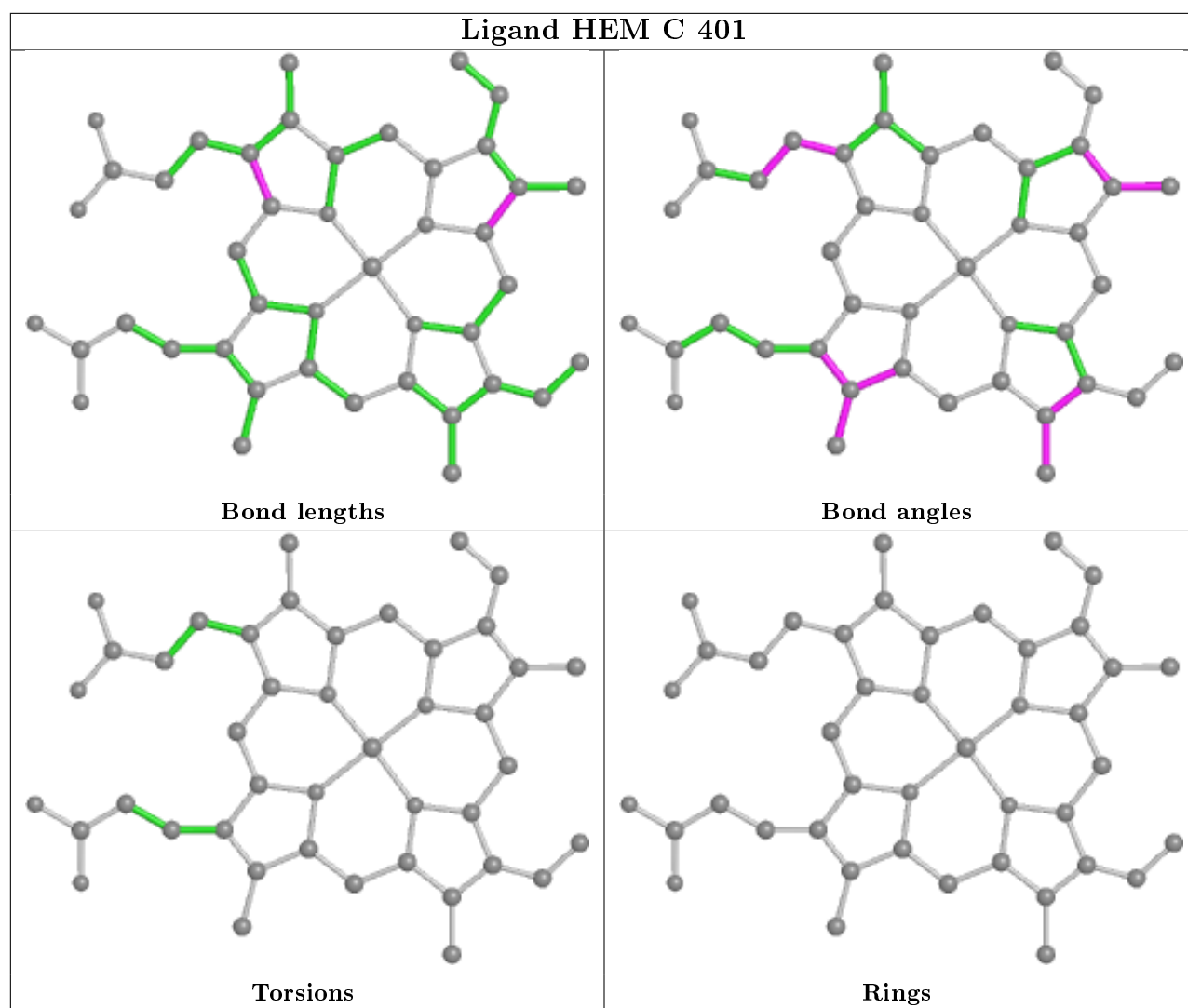


Torsions

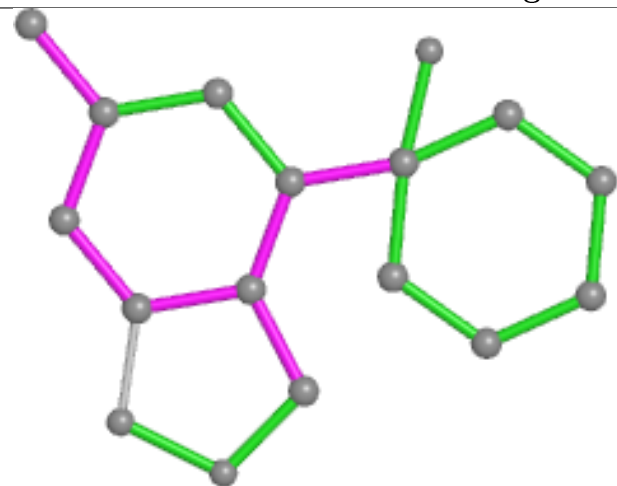


Rings

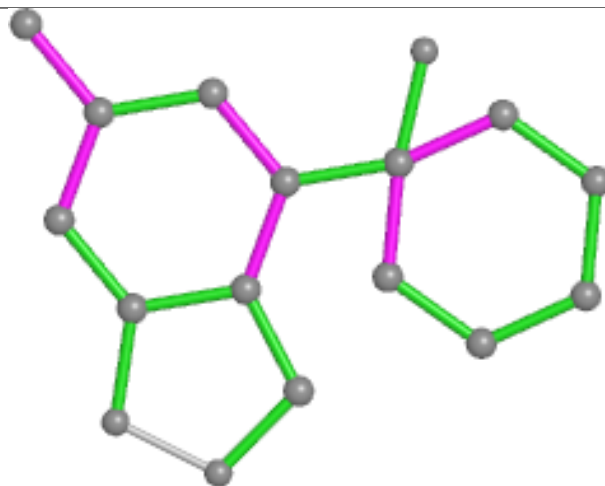




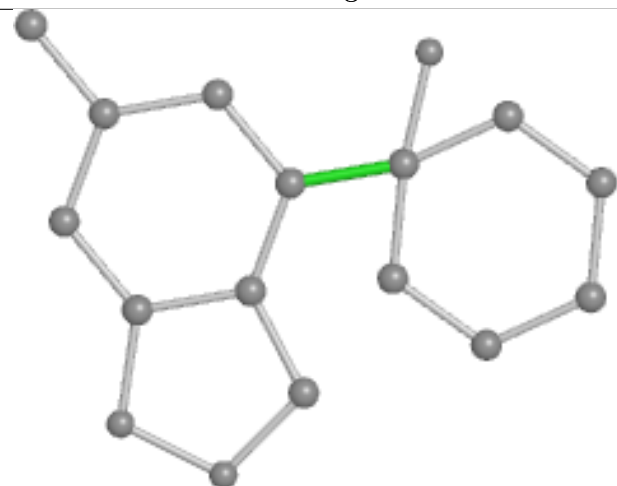
Ligand 9R9 A 402



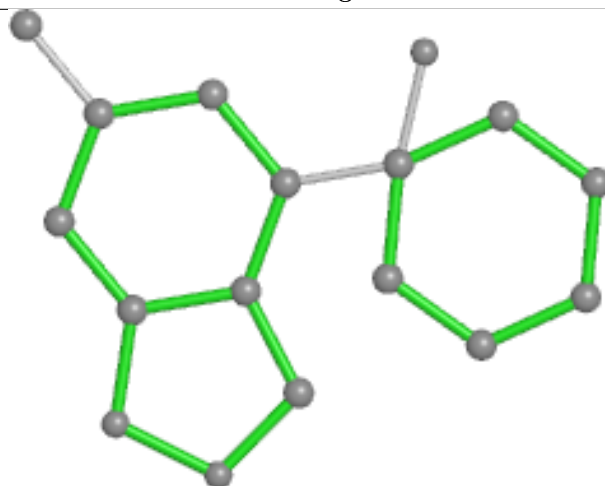
Bond lengths



Bond angles

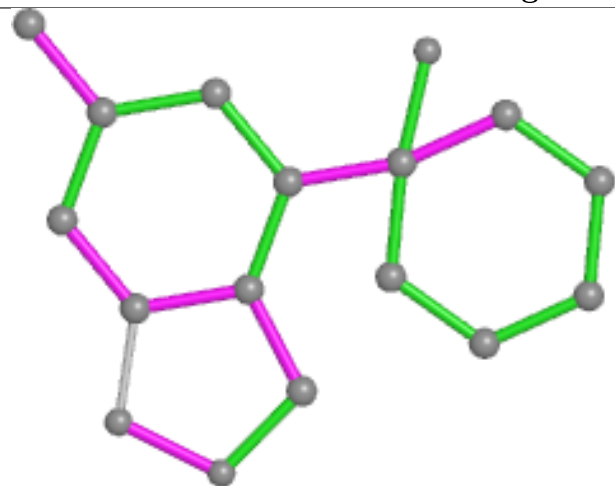


Torsions

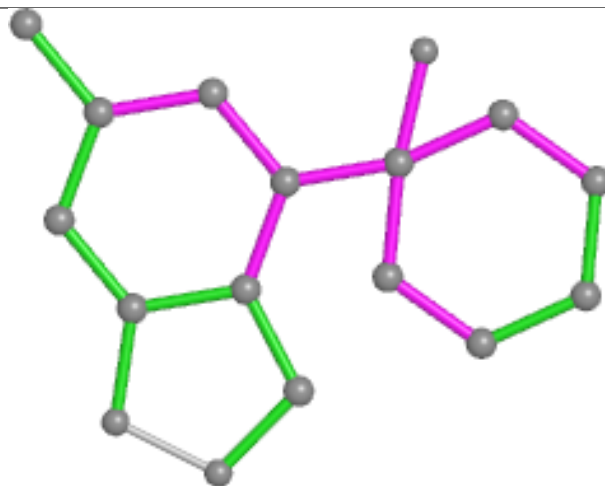


Rings

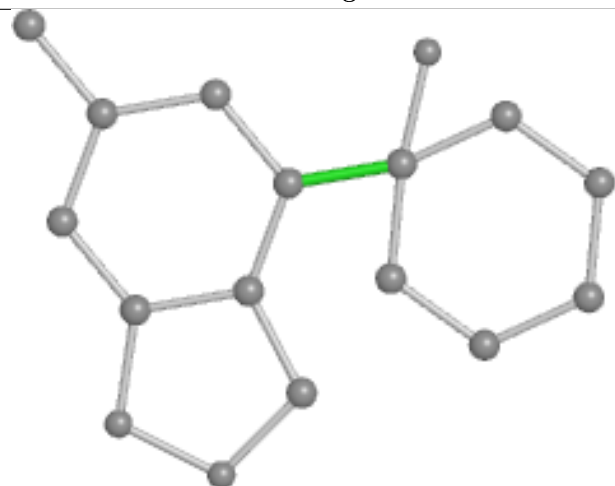
Ligand 9R9 D 402



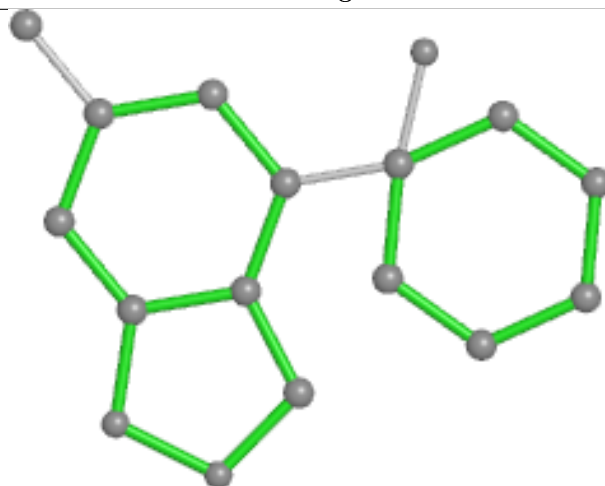
Bond lengths



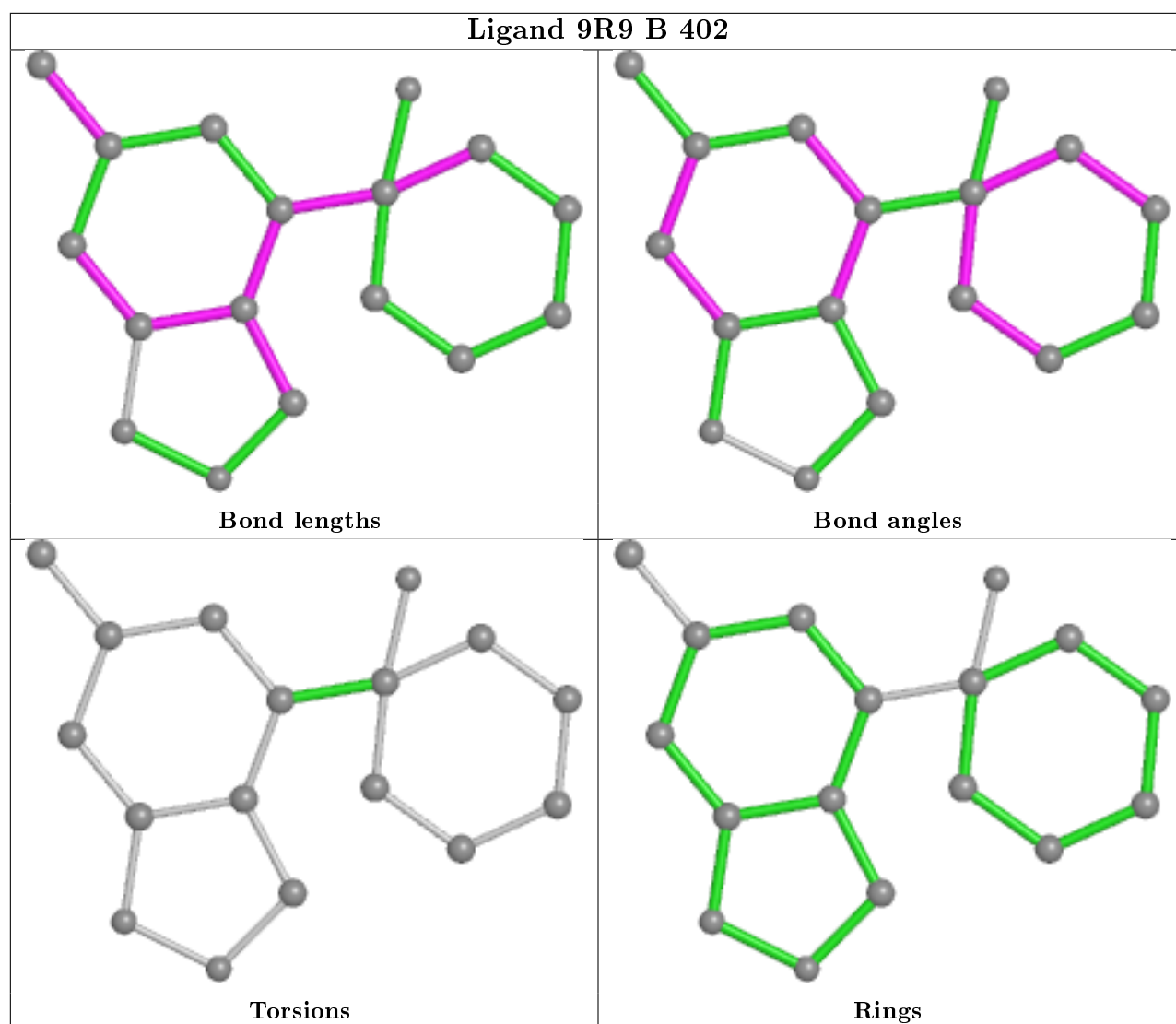
Bond angles



Torsions



Rings



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	322/391 (82%)	0.06	7 (2%) 62 57	47, 68, 118, 168	0
1	B	309/391 (79%)	0.12	17 (5%) 25 21	50, 84, 139, 190	0
1	C	323/391 (82%)	0.34	25 (7%) 13 10	58, 97, 146, 170	0
1	D	290/391 (74%)	0.33	27 (9%) 8 7	55, 97, 148, 169	0
All	All	1244/1564 (79%)	0.21	76 (6%) 21 18	47, 86, 144, 190	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	264	LEU	6.8
1	A	345	SER	6.3
1	C	254	VAL	5.6
1	D	265	LEU	5.0
1	D	218	HIS	4.9
1	D	193	LEU	4.8
1	C	220	PHE	4.8
1	D	268	PHE	4.7
1	C	173	VAL	4.6
1	C	215	LEU	4.3
1	D	192	LEU	4.2
1	D	190	GLU	4.1
1	D	275	HIS	4.1
1	B	191	LEU	3.9
1	D	371	TYR	3.9
1	D	62	LYS	3.8
1	B	381	MET	3.8
1	D	217	PRO	3.7
1	C	255	ALA	3.7
1	B	347	GLY	3.7
1	D	276	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	273	HIS	3.5
1	C	241	ILE	3.4
1	D	219	GLY	3.4
1	D	272	ARG	3.4
1	B	263	VAL	3.4
1	D	263	VAL	3.3
1	C	223	TRP	3.2
1	B	236	GLU	3.1
1	A	170	ASN	3.1
1	D	197	GLN	3.1
1	A	41	ILE	3.0
1	B	351	LEU	3.0
1	D	267	LEU	3.0
1	C	313	SER	2.9
1	A	344	GLY	2.9
1	D	278	SER	2.9
1	C	169	GLN	2.8
1	A	346	SER	2.8
1	C	171	MET	2.8
1	D	196	GLU	2.7
1	D	58	GLN	2.6
1	B	226	LEU	2.6
1	B	265	LEU	2.6
1	D	146	TYR	2.6
1	B	149	PRO	2.6
1	B	220	PHE	2.6
1	C	272	ARG	2.6
1	C	262	GLU	2.6
1	C	259	LYS	2.5
1	C	338	SER	2.5
1	C	371	TYR	2.5
1	C	290	GLN	2.5
1	C	265	LEU	2.5
1	D	188	GLU	2.5
1	C	217	PRO	2.3
1	D	189	ASN	2.3
1	B	349	HIS	2.3
1	B	382	ASN	2.2
1	C	286	TYR	2.2
1	D	271	LYS	2.2
1	C	222	PHE	2.2
1	B	119	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	119	SER	2.2
1	C	213	PRO	2.2
1	D	274	GLU	2.2
1	A	240	ARG	2.2
1	C	214	GLY	2.1
1	B	254	VAL	2.1
1	B	186	GLY	2.1
1	C	284	LEU	2.1
1	B	259	LYS	2.1
1	A	119	SER	2.1
1	D	191	LEU	2.0
1	C	116	HIS	2.0
1	B	350	TYR	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 monosaccharides 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(\AA^2)	Q<0.9
5	CIT	A	404	13/13	0.67	0.24	90,121,135,140	0
2	HEM	B	401	43/43	0.96	0.22	68,76,98,107	0
4	TRP	D	403	15/15	0.96	0.13	83,90,109,117	0
2	HEM	D	401	43/43	0.97	0.17	78,88,107,109	0
3	9R9	C	402	17/17	0.97	0.12	61,69,78,92	0
3	9R9	D	402	17/17	0.97	0.12	69,74,84,91	0
4	TRP	B	403	15/15	0.97	0.15	56,66,76,83	0
3	9R9	A	402	17/17	0.98	0.13	49,53,69,70	0
2	HEM	A	401	43/43	0.98	0.16	51,61,82,92	0
2	HEM	C	401	43/43	0.98	0.18	70,80,105,111	0

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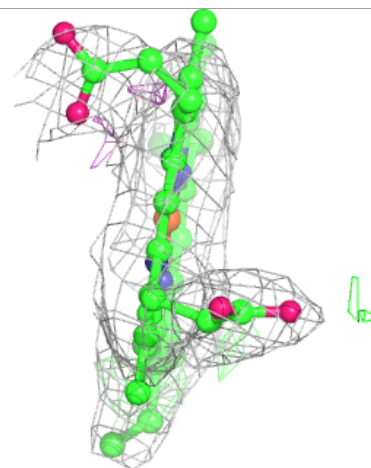
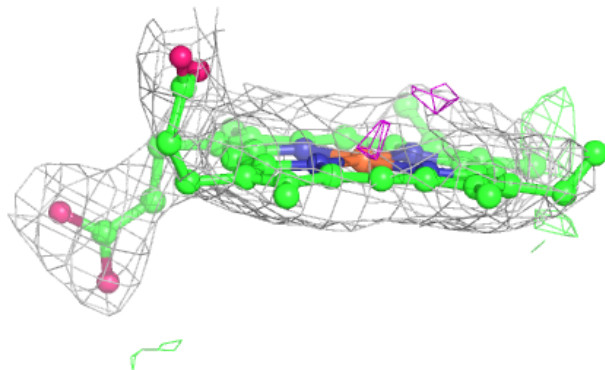
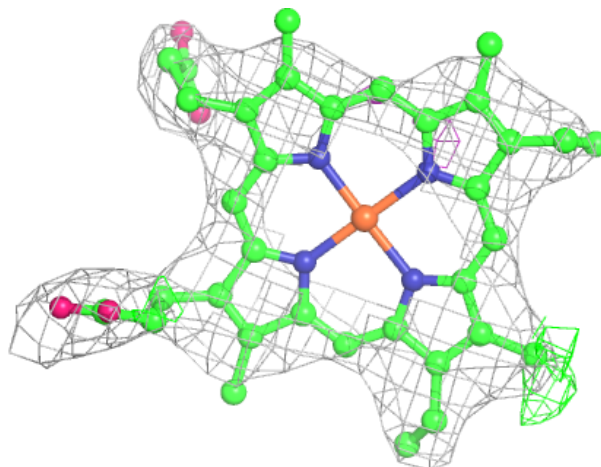
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	9R9	B	402	17/17	0.98	0.13	63,66,70,82	0
4	TRP	A	403	15/15	0.98	0.15	52,57,68,72	0

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.

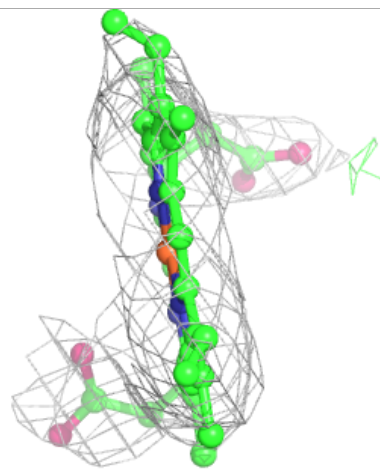
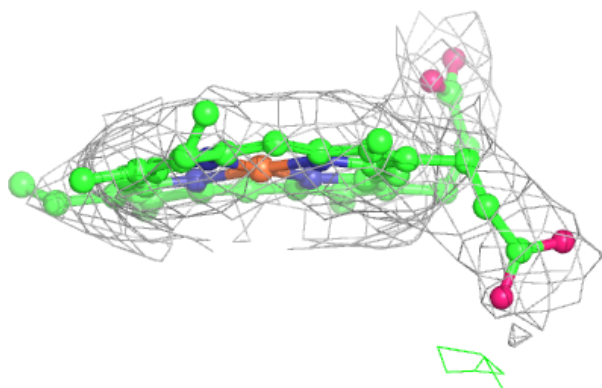
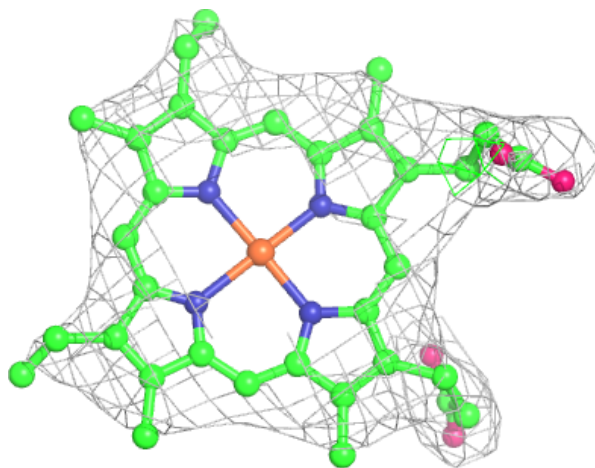
Electron density around HEM B 401:

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



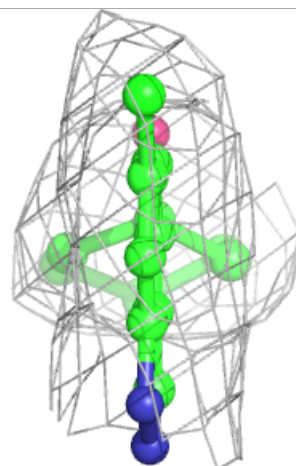
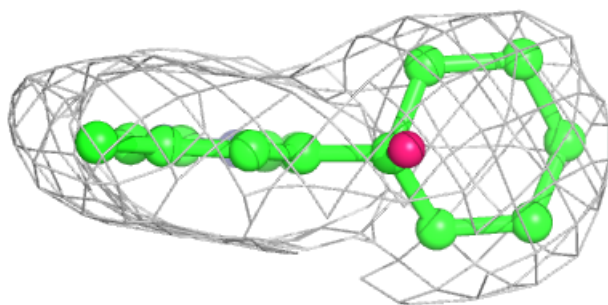
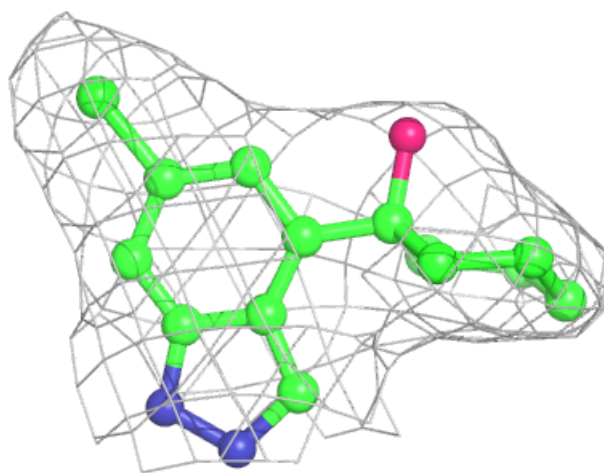
Electron density around HEM D 401:

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



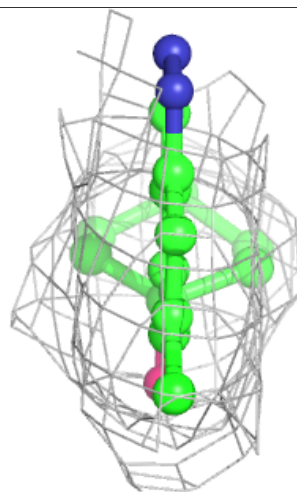
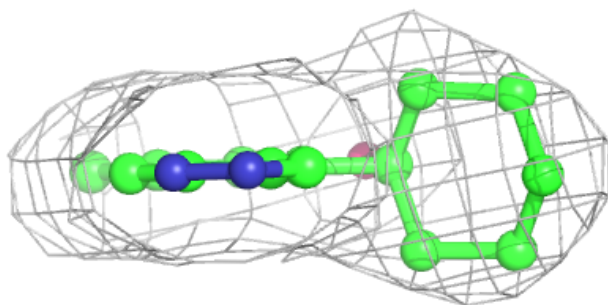
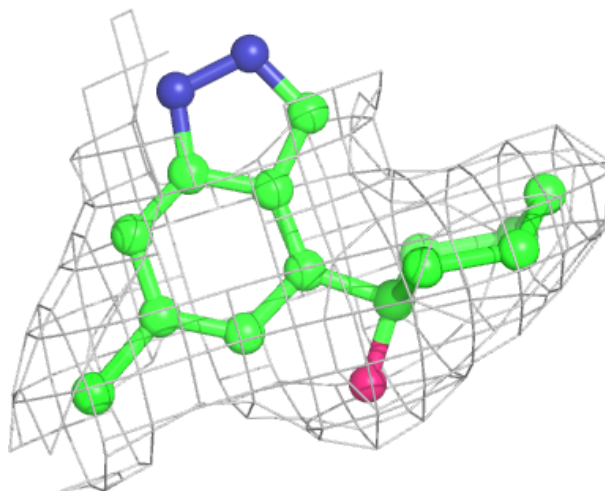
Electron density around 9R9 C 402:

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



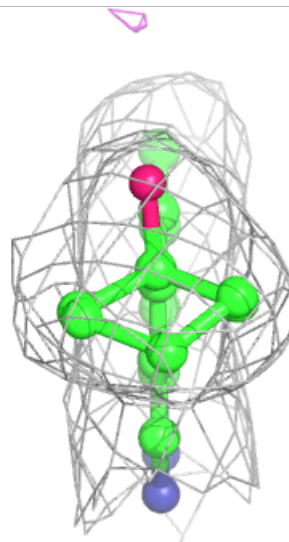
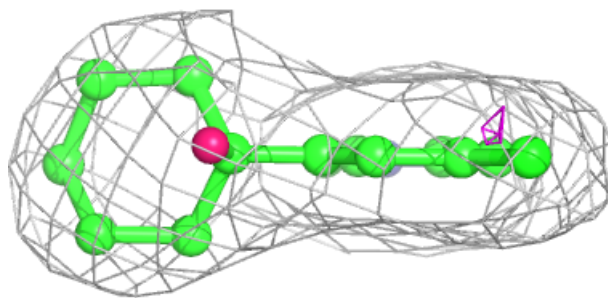
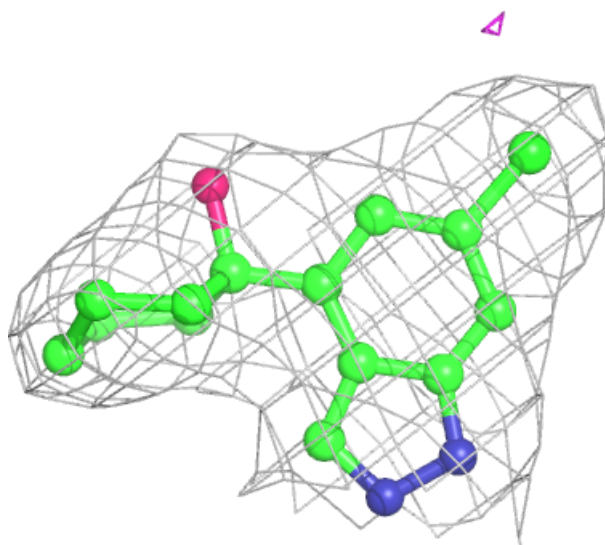
Electron density around 9R9 D 402:

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



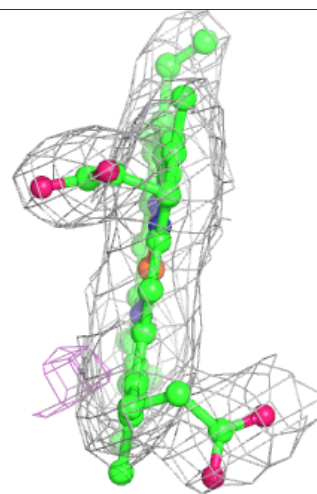
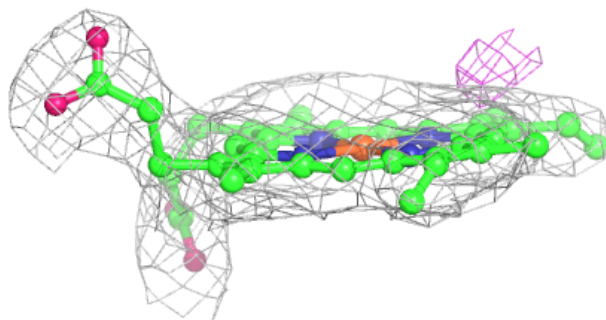
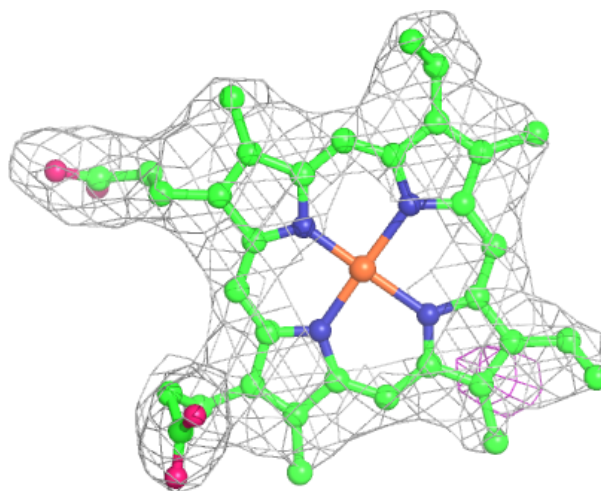
Electron density around 9R9 A 402:

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



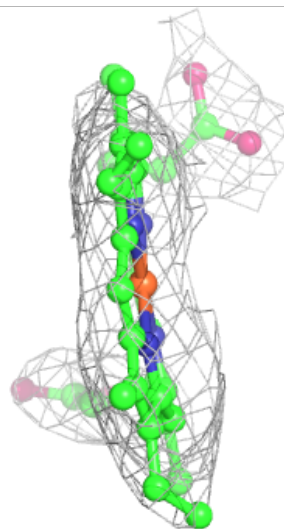
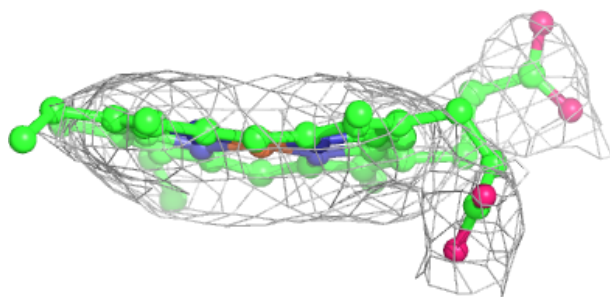
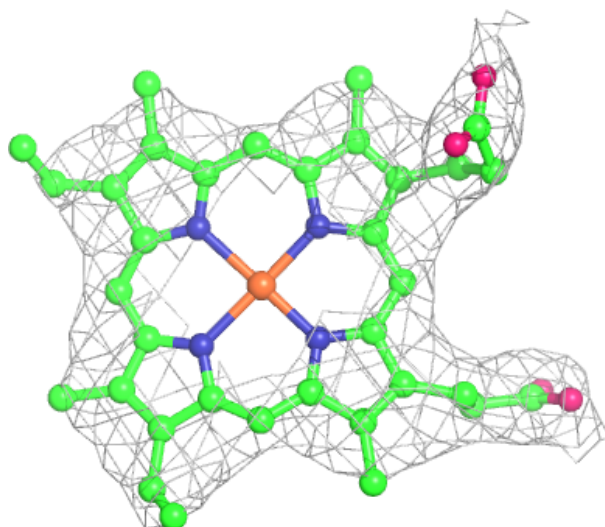
Electron density around HEM A 401:

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



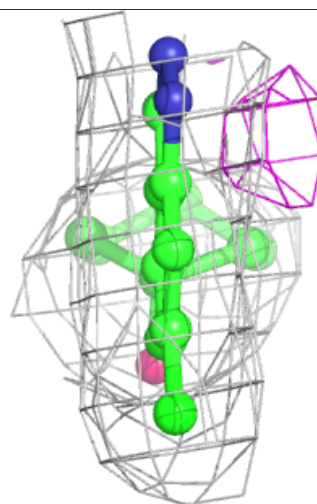
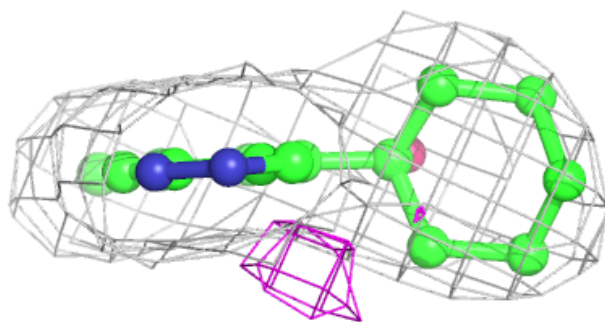
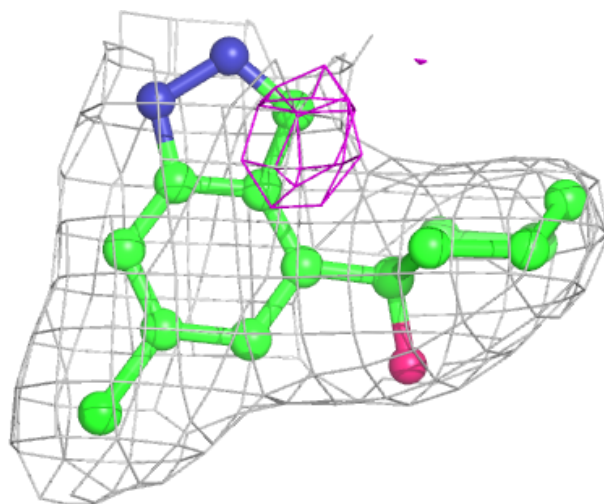
Electron density around HEM C 401:

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



Electron density around 9R9 B 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.