



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:04 AM JST

PDB ID : 6A4I / pdb_00006a4i
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

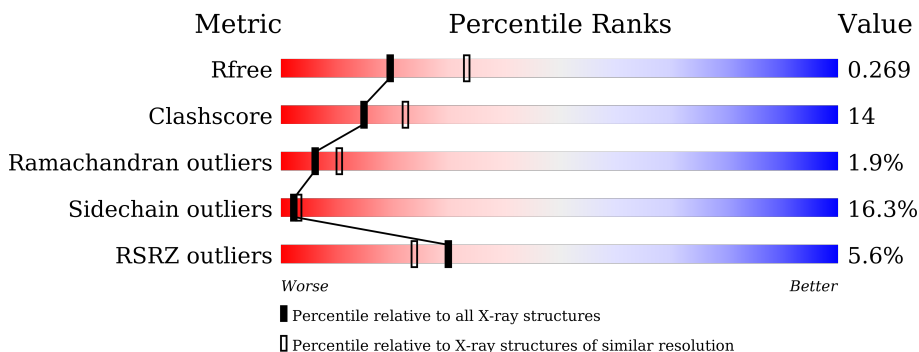
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	3% 53% 21% 7% • 18%
1	B	391	3% 46% 24% 8% • 21%
1	C	391	4% 50% 23% 8% • 17%
1	D	391	7% 39% 26% 7% • 26%

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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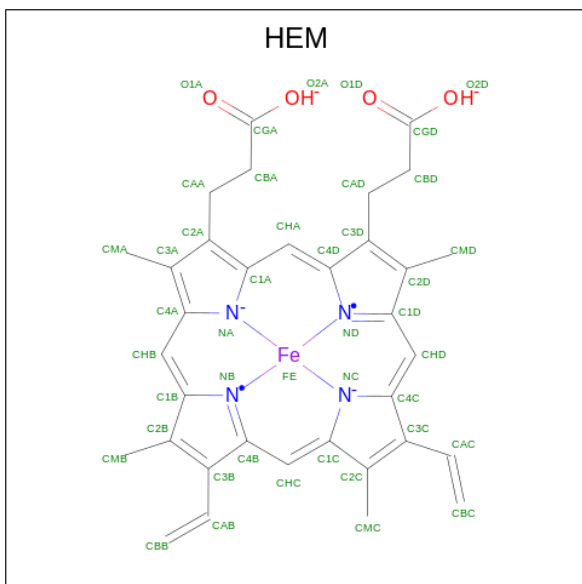
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B	-2	MET	-	expression tag	UNP P48775
B	-1	GLY	-	expression tag	UNP P48775
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B	1	SER	-	expression tag	UNP P48775
B	2	HIS	-	expression tag	UNP P48775
B	3	HIS	-	expression tag	UNP P48775
B	4	HIS	-	expression 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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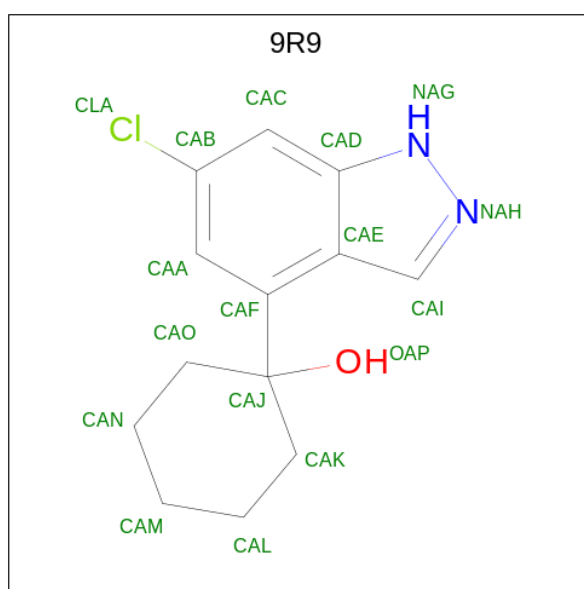
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP P48775
D	-1	GLY	-	expression tag	UNP P48775
D	0	SER	-	expression tag	UNP P48775
D	1	SER	-	expression tag	UNP P48775
D	2	HIS	-	expression tag	UNP P48775
D	3	HIS	-	expression tag	UNP P48775
D	4	HIS	-	expression tag	UNP P48775
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 (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



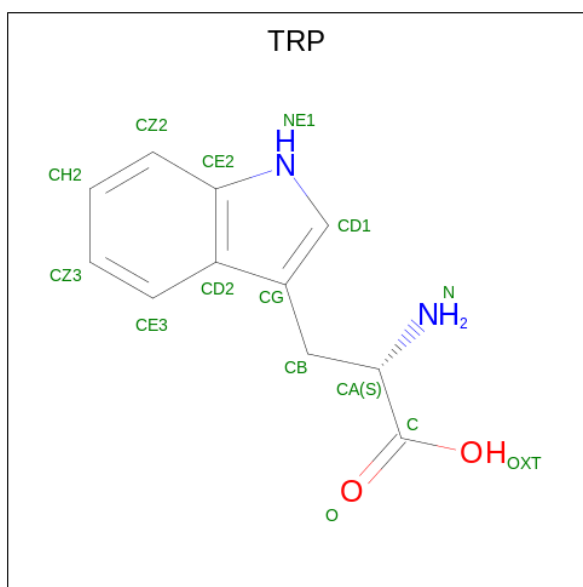
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



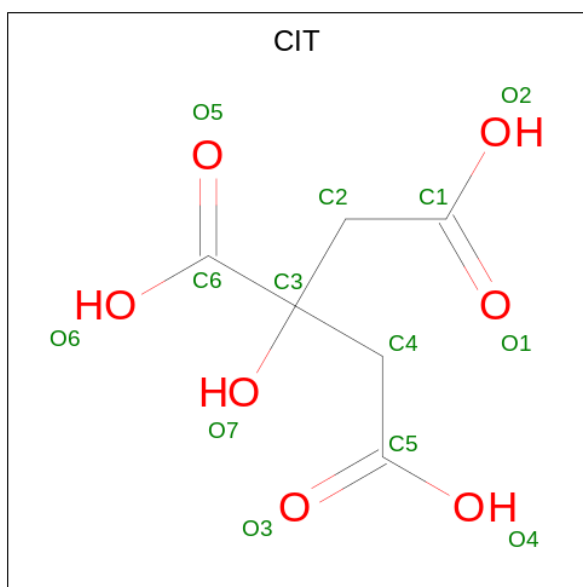
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
3	C	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
3	D	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		

- Molecule 4 is TRYPTOPHAN (CCD ID: 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 (CCD ID: CIT) (formula: $C_6H_8O_7$).

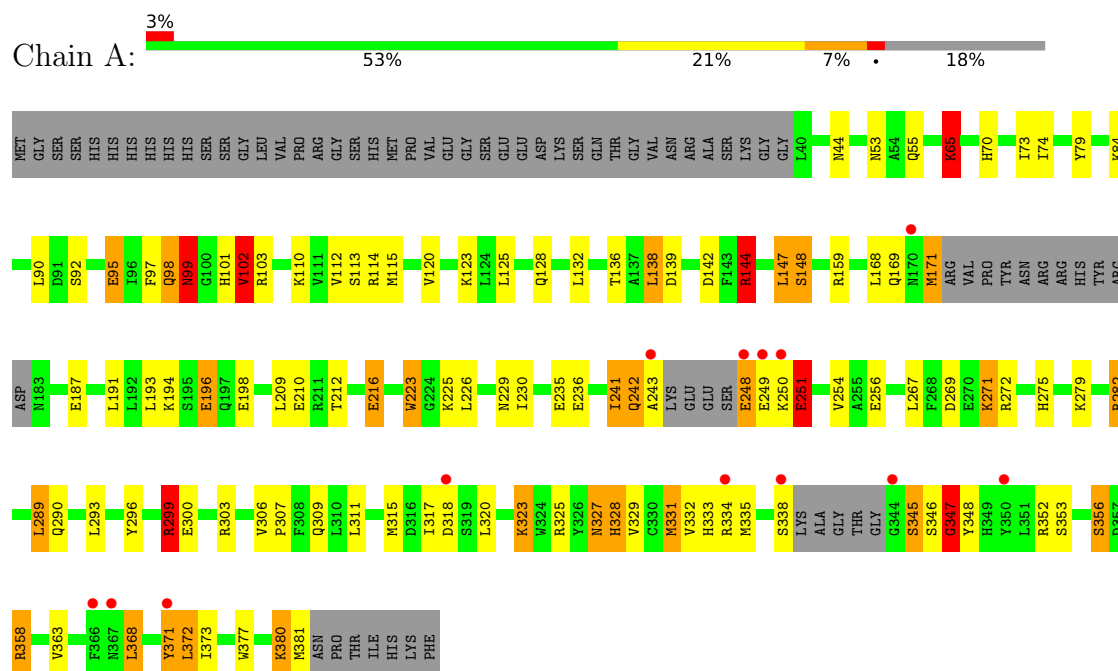


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

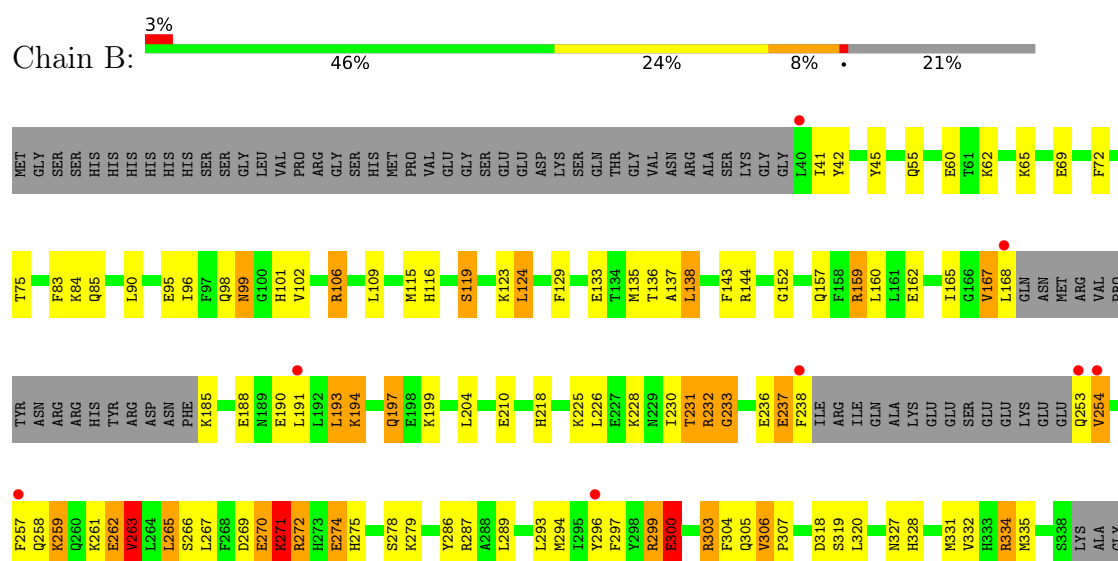
3 Residue-property plots

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

• Molecule 1: Tryptophan 2,3-dioxygenase

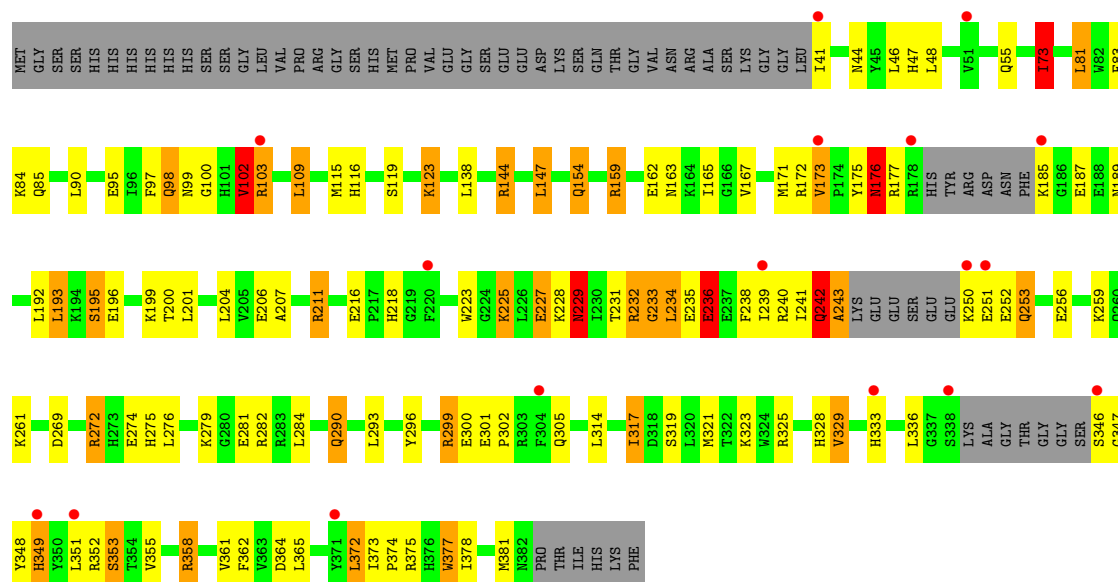


• Molecule 1: Tryptophan 2,3-dioxygenase

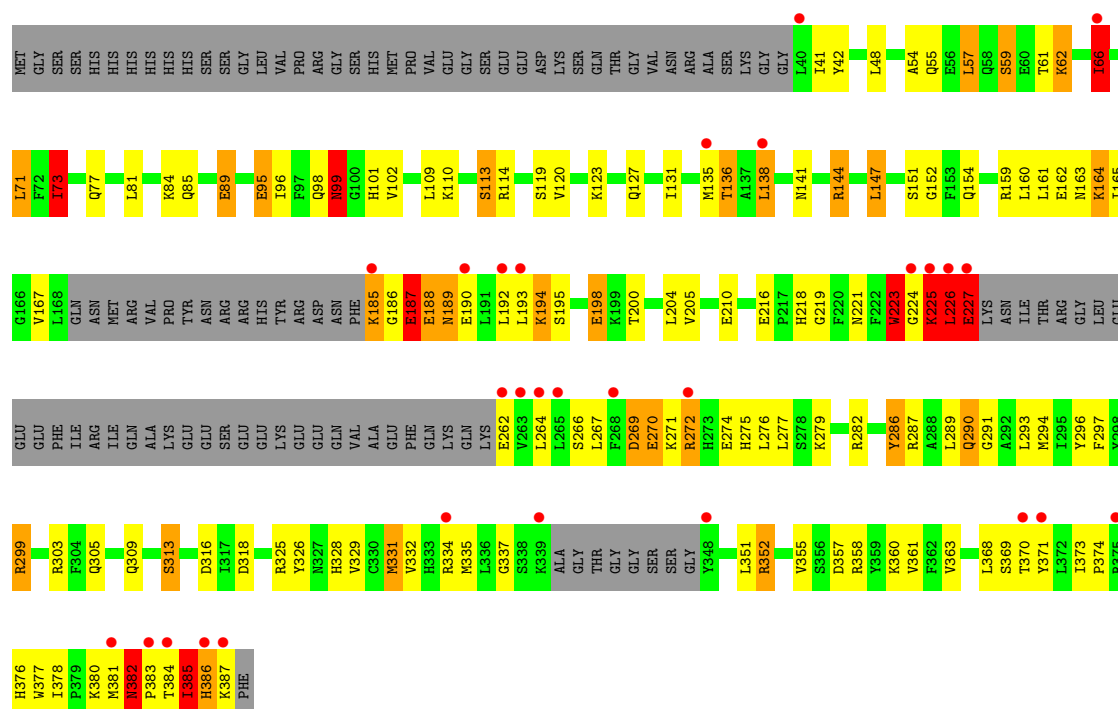




• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase



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 – 2.65 105.95 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (106.17-2.65) 99.9 (105.95-2.65)	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 , 0.269	Depositor DCC
R_{free} test set	3058 reflections (5.13%)	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)	0.30 , 47.2	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: 9R9, HEM, CIT

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	1.54	25/2769 (0.9%)	1.51	27/3723 (0.7%)
1	B	1.40	15/2668 (0.6%)	1.41	19/3592 (0.5%)
1	C	1.49	27/2782 (1.0%)	1.45	20/3743 (0.5%)
1	D	1.59	38/2521 (1.5%)	1.48	25/3395 (0.7%)
All	All	1.50	105/10740 (1.0%)	1.46	91/14453 (0.6%)

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 (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	GLU	N-CA	20.14	1.84	1.46
1	C	243	ALA	N-CA	17.10	1.78	1.46
1	C	243	ALA	CA-C	-14.51	1.22	1.52
1	D	270	GLU	CA-C	14.50	1.71	1.52
1	C	232	ARG	CB-CG	12.44	1.89	1.52
1	B	254	VAL	CA-CB	11.84	1.68	1.54
1	B	218	HIS	CD2-NE2	11.47	1.50	1.37
1	C	374	PRO	N-CD	11.24	1.63	1.47
1	B	237	GLU	C-N	10.96	1.48	1.33
1	D	274	GLU	C-O	10.87	1.37	1.24
1	D	282	ARG	NE-CZ	10.41	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	PHE	CG-CD1	9.72	1.59	1.38
1	D	271	LYS	N-CA	9.54	1.57	1.46
1	C	227	GLU	CB-CG	9.10	1.79	1.52
1	A	250	LYS	C-O	8.89	1.34	1.23
1	C	239	ILE	CA-CB	8.85	1.67	1.54
1	A	250	LYS	N-CA	8.59	1.57	1.46
1	D	286	TYR	CE1-CZ	8.54	1.58	1.38
1	B	237	GLU	C-O	8.43	1.33	1.24
1	D	286	TYR	CG-CD1	8.43	1.57	1.39
1	D	189	ASN	CG-OD1	8.09	1.39	1.23
1	D	270	GLU	C-N	8.09	1.43	1.33
1	A	243	ALA	C-O	7.98	1.39	1.23
1	D	198	GLU	N-CA	7.92	1.55	1.45
1	A	248	GLU	CA-CB	-7.87	1.37	1.53
1	D	275	HIS	CD2-NE2	7.78	1.46	1.37
1	D	382	ASN	CA-C	7.74	1.62	1.52
1	B	233	GLY	N-CA	7.71	1.56	1.45
1	B	236	GLU	CD-OE2	7.59	1.39	1.25
1	A	249	GLU	CG-CD	7.50	1.70	1.52
1	C	242	GLN	CA-C	7.40	1.62	1.52
1	C	233	GLY	N-CA	7.18	1.54	1.45
1	D	270	GLU	N-CA	-7.07	1.38	1.46
1	D	262	GLU	C-N	7.07	1.43	1.33
1	D	194	LYS	N-CA	6.95	1.54	1.46
1	A	371	TYR	N-CA	6.90	1.54	1.46
1	D	271	LYS	CA-C	6.78	1.62	1.52
1	D	384	THR	CA-CB	6.73	1.61	1.53
1	D	73	ILE	CA-CB	6.67	1.62	1.54
1	C	235	GLU	CG-CD	-6.67	1.35	1.52
1	A	98	GLN	C-O	-6.41	1.16	1.24
1	D	189	ASN	CG-ND2	6.35	1.46	1.33
1	C	238	PHE	CA-C	6.32	1.61	1.52
1	C	235	GLU	CD-OE1	-6.28	1.13	1.25
1	C	173	VAL	CA-C	6.26	1.59	1.52
1	D	381	MET	CA-C	6.25	1.59	1.52
1	A	251	GLU	CD-OE2	6.22	1.37	1.25
1	C	229	ASN	CA-C	6.20	1.60	1.52
1	C	240	ARG	C-O	6.17	1.31	1.24
1	D	198	GLU	CA-CB	-6.09	1.43	1.53
1	B	119	SER	N-CA	-5.97	1.38	1.46
1	D	382	ASN	C-N	5.86	1.39	1.33
1	D	282	ARG	CD-NE	5.84	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	144	ARG	CZ-NH2	5.79	1.41	1.33
1	C	275	HIS	CE1-NE2	5.71	1.38	1.32
1	A	315	MET	N-CA	-5.71	1.38	1.46
1	B	45	TYR	C-O	-5.65	1.17	1.24
1	B	231	THR	CB-OG1	5.65	1.52	1.43
1	D	227	GLU	N-CA	5.64	1.56	1.46
1	A	248	GLU	C-N	5.64	1.41	1.33
1	C	377	TRP	CD2-CE2	-5.63	1.31	1.41
1	A	289	LEU	N-CA	-5.58	1.39	1.46
1	B	319	SER	C-O	5.57	1.30	1.24
1	D	218	HIS	CB-CG	5.57	1.57	1.50
1	D	274	GLU	CA-C	5.53	1.60	1.52
1	A	210	GLU	C-O	-5.53	1.16	1.24
1	B	218	HIS	CG-ND1	5.51	1.44	1.38
1	D	384	THR	N-CA	5.50	1.53	1.46
1	B	185	LYS	C-N	5.49	1.40	1.33
1	A	320	LEU	N-CA	-5.48	1.39	1.46
1	C	239	ILE	N-CA	5.46	1.53	1.46
1	C	239	ILE	CA-C	5.45	1.60	1.52
1	D	269	ASP	CA-CB	5.41	1.60	1.52
1	C	231	THR	CA-C	-5.39	1.45	1.52
1	C	236	GLU	CG-CD	5.34	1.65	1.52
1	D	185	LYS	C-O	5.34	1.34	1.23
1	A	223	TRP	CA-C	-5.33	1.45	1.52
1	A	345	SER	N-CA	5.33	1.53	1.46
1	D	275	HIS	CG-CD2	-5.32	1.29	1.35
1	D	193	LEU	N-CA	5.32	1.52	1.46
1	A	368	LEU	C-O	5.30	1.30	1.24
1	D	194	LYS	CD-CE	5.29	1.68	1.52
1	A	73	ILE	C-O	-5.24	1.18	1.24
1	C	377	TRP	NE1-CE2	-5.24	1.31	1.37
1	D	223	TRP	CZ2-CH2	5.22	1.47	1.37
1	A	306	VAL	CA-CB	-5.22	1.50	1.53
1	C	73	ILE	CA-CB	5.22	1.60	1.54
1	C	323	LYS	CA-C	5.21	1.59	1.52
1	D	270	GLU	CD-OE2	5.20	1.35	1.25
1	D	382	ASN	N-CA	5.17	1.53	1.46
1	A	363	VAL	N-CA	-5.17	1.40	1.46
1	B	300	GLU	CA-C	5.17	1.59	1.52
1	C	232	ARG	C-O	-5.16	1.18	1.24
1	D	384	THR	CA-C	5.16	1.59	1.52
1	A	74	ILE	CA-CB	5.12	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	386	HIS	CA-C	5.12	1.59	1.53
1	C	103	ARG	CD-NE	5.11	1.53	1.46
1	A	254	VAL	CA-CB	5.08	1.60	1.54
1	A	212	THR	N-CA	5.07	1.51	1.45
1	A	235	GLU	N-CA	5.06	1.52	1.46
1	D	226	LEU	C-N	5.05	1.40	1.33
1	C	349	HIS	N-CA	5.05	1.52	1.46
1	B	116	HIS	C-O	5.04	1.30	1.24
1	A	282	ARG	NE-CZ	5.03	1.38	1.33
1	C	225	LYS	CA-C	5.02	1.59	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	VAL	N-CA-CB	14.09	128.08	110.47
1	D	381	MET	N-CA-C	10.96	127.23	113.43
1	C	243	ALA	CA-C-O	10.43	138.53	120.80
1	A	248	GLU	N-CA-CB	-9.88	93.71	110.50
1	A	251	GLU	N-CA-C	-9.78	99.69	114.16
1	C	102	VAL	CB-CA-C	-9.55	99.04	112.22
1	B	271	LYS	N-CA-C	8.62	121.46	111.11
1	D	194	LYS	CG-CD-CE	8.25	130.28	111.30
1	D	370	THR	N-CA-C	-8.13	103.82	114.31
1	C	377	TRP	CG-CD1-NE1	-8.08	99.70	110.20
1	D	59	SER	N-CA-C	-7.86	103.52	113.43
1	A	102	VAL	CB-CA-C	-7.84	96.81	111.79
1	C	123	LYS	N-CA-C	-7.79	102.87	111.36
1	B	218	HIS	CE1-NE2-CD2	7.77	116.77	109.00
1	B	218	HIS	ND1-CE1-NE2	-7.64	100.76	108.40
1	C	235	GLU	CB-CG-CD	-7.43	99.97	112.60
1	A	325	ARG	N-CA-C	-7.35	103.34	111.36
1	A	372	LEU	N-CA-C	7.34	121.03	110.24
1	B	306	VAL	CA-C-N	-7.16	112.26	119.56
1	B	306	VAL	C-N-CA	-7.16	112.26	119.56
1	B	99	ASN	N-CA-C	-7.16	104.70	113.50
1	C	73	ILE	N-CA-CB	7.01	118.57	110.65
1	B	218	HIS	CG-CD2-NE2	-6.96	100.24	107.20
1	C	234	LEU	N-CA-C	6.89	118.58	111.14
1	D	120	VAL	N-CA-C	-6.88	103.77	110.72
1	D	384	THR	N-CA-C	6.83	119.41	108.41
1	B	99	ASN	N-CA-CB	-6.73	100.64	110.53
1	D	282	ARG	CG-CD-NE	6.71	126.76	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASN	N-CA-C	6.70	118.67	111.36
1	D	269	ASP	O-C-N	-6.68	114.50	122.46
1	D	198	GLU	N-CA-C	-6.46	101.38	110.50
1	A	328	HIS	N-CA-C	-6.45	104.17	111.14
1	D	286	TYR	CD1-CE1-CZ	-6.42	108.04	119.60
1	B	237	GLU	O-C-N	6.41	129.01	122.09
1	A	95	GLU	N-CA-C	6.40	118.26	111.28
1	B	297	PHE	N-CA-C	6.40	118.26	111.28
1	D	147	LEU	N-CA-C	-6.37	106.05	113.88
1	A	99	ASN	CB-CA-C	-6.33	97.82	110.42
1	D	114	ARG	N-CA-C	6.33	118.26	111.36
1	A	120	VAL	N-CA-C	-6.26	103.05	111.44
1	B	254	VAL	CA-CB-CG1	6.24	121.01	110.40
1	D	291	GLY	N-CA-C	-6.20	105.31	112.50
1	B	294	MET	N-CA-C	-6.19	104.46	111.14
1	B	75	THR	N-CA-C	-6.17	104.47	111.07
1	A	299	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	C	352	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	D	66	ILE	CB-CA-C	6.14	118.39	110.96
1	A	216	GLU	CA-C-N	-6.11	113.33	119.56
1	A	216	GLU	C-N-CA	-6.11	113.33	119.56
1	C	103	ARG	CB-CG-CD	6.10	125.34	111.30
1	B	263	VAL	N-CA-CB	6.09	119.72	110.58
1	A	249	GLU	CA-C-N	-6.08	113.48	122.41
1	A	249	GLU	C-N-CA	-6.08	113.48	122.41
1	D	305	GLN	N-CA-C	6.05	118.40	111.02
1	D	294	MET	N-CA-C	-6.05	104.02	111.40
1	C	204	LEU	N-CA-C	6.04	117.86	111.28
1	C	253	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	B	83	PHE	N-CA-C	-5.96	104.78	111.28
1	C	377	TRP	CZ3-CH2-CZ2	-5.89	113.84	121.50
1	D	270	GLU	CA-C-O	-5.89	114.64	120.82
1	D	189	ASN	O-C-N	5.87	130.50	122.46
1	D	163	ASN	N-CA-C	5.84	117.45	111.14
1	C	355	VAL	N-CA-C	-5.76	106.88	112.29
1	D	318	ASP	N-CA-C	5.74	117.21	111.07
1	A	306	VAL	O-C-N	5.67	124.09	120.07
1	C	81	LEU	N-CA-C	-5.66	105.11	111.28
1	D	382	ASN	N-CA-C	5.64	122.28	109.81
1	D	66	ILE	N-CA-CB	5.60	117.38	111.00
1	B	362	PHE	N-CA-C	5.55	118.84	112.57
1	A	103	ARG	NE-CZ-NH2	5.49	124.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	GLU	CA-C-N	5.40	126.59	119.84
1	C	216	GLU	C-N-CA	5.40	126.59	119.84
1	D	189	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	A	139	ASP	N-CA-CB	5.32	118.03	110.16
1	A	148	SER	N-CA-CB	5.32	118.06	110.03
1	D	89	GLU	N-CA-C	-5.31	105.57	111.36
1	C	346	SER	CA-C-N	5.25	125.78	120.00
1	C	346	SER	C-N-CA	5.25	125.78	120.00
1	A	112	VAL	N-CA-C	5.25	115.97	110.62
1	A	65	LYS	CB-CG-CD	5.24	123.35	111.30
1	A	356	SER	N-CA-C	5.17	117.48	110.35
1	A	113	SER	CA-CB-OG	-5.11	100.87	111.10
1	B	167	VAL	N-CA-CB	5.10	118.35	110.14
1	C	163	ASN	N-CA-C	5.09	116.91	111.36
1	A	254	VAL	CG1-CB-CG2	-5.07	99.64	110.80
1	C	229	ASN	N-CA-C	5.07	116.81	111.28
1	D	99	ASN	CB-CA-C	-5.06	100.36	110.42
1	A	144	ARG	CA-C-N	5.03	127.02	120.28
1	A	144	ARG	C-N-CA	5.03	127.02	120.28
1	A	323	LYS	N-CA-C	-5.02	105.89	111.36
1	B	320	LEU	N-CA-C	-5.01	105.53	111.69

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	59	0
1	B	2608	0	2605	90	0
1	C	2722	0	2714	81	0
1	D	2463	0	2470	90	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
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	295	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 14.

All (295) 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:CG	1:C:227:GLU:CB	1.79	1.60
1:C:232:ARG:CB	1:C:232:ARG:CG	1.89	1.50
1:C:243:ALA:N	1:C:243:ALA:CA	1.78	1.45
1:A:248:GLU:CA	1:A:248:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:243:ALA:N	1:C:243:ALA:C	2.41	0.79
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
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:HD22	1:D:57:LEU:H	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:115:MET:HE3	1:A:317:ILE:CD1	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:242:GLN:C	1:C:243:ALA:CA	2.67	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
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:98:GLN:C	1:C:100:GLY:H	2.07	0.63
1:C:362:PHE:HB3	1:C:365:LEU:HD12	1.81	0.63
1:B:133:GLU:HB3	1:B:334:ARG:NH2	2.11	0.63
1:B:269:ASP:CB	1:B:272:ARG:HH22	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:D:135:MET:HE3	1:D:335:MET:HE3	1.85	0.59
1:B:300:GLU:OE1	1:B:300:GLU:N	2.27	0.58
1:B:296:TYR:O	1:B:299:ARG:NH1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:259:LYS:HA	1:B:262:GLU:CD	2.29	0.57
1:D:286:TYR:O	1:D:289:LEU:HB3	2.04	0.57
1:C:85:GLN:CD	1:D:71:LEU:HD22	2.30	0.57
1:A:144:ARG:O	1:A:147:LEU:HB2	2.05	0.56
1:D:187:GLU:C	1:D:189:ASN:H	2.13	0.56
1:D:187:GLU:C	1:D:189:ASN:N	2.61	0.56
1:A:92:SER:OG	1:A:114:ARG:NH1	2.39	0.56
1:A:115:MET:HE3	1:A:317:ILE:HD12	1.87	0.56
1:A:142:ASP:CG	1:C:375:ARG:HE	2.14	0.56
1:B:84:LYS:HG3	1:B:157:GLN:HE22	1.71	0.55
1:C:227:GLU:CG	1:C:227:GLU:CA	2.76	0.55
1:A:296:TYR:HE2	1:A:368:LEU:HB2	1.72	0.55
1:C:47:HIS:HB2	1:D:54:ALA:HB1	1.86	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: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:C:227:GLU:CB	1:C:227:GLU:CD	2.73	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:D:303:ARG:NH1	1:D:385:ILE:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:MET:HE3	1:C:317:ILE:HD13	1.91	0.52
1:C:229:ASN:HD21	1:C:232:ARG:NH2	2.05	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
1:C:272:ARG:HH11	1:C:276:LEU:HD11	1.75	0.52
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:A:171:MET:HE1	1:A:358:ARG:HH11	1.75	0.51
1:C:175:TYR:O	1:C:176:ASN:HB2	2.10	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:59:SER:HB3	1:D:66:ILE:H	1.77	0.50
1:D:98:GLN:HG3	1:D:204:LEU:HD21	1.94	0.50
1:A:65:LYS:NZ	1:A:65:LYS:H	2.09	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:C:301:GLU:O	1:C:302:PRO:C	2.56	0.48
1:A:269:ASP:CG	1:A:272:ARG:HB2	2.38	0.48
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:D:95:GLU:O	1:D:99:ASN:HB2	2.14	0.48
1:A:248:GLU:N	1:A:248:GLU:C	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ILE:C	1:C:243:ALA:H	2.22	0.48
1:B:269:ASP:O	1:B:270:GLU:C	2.57	0.48
1:D:96:ILE:C	1:D:102:VAL:HG23	2.38	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:D:269:ASP:CG	1:D:272:ARG:HB2	2.39	0.47
1:B:159:ARG:NH1	2:B:401:HEM:O2D	2.28	0.47
1:B:303:ARG:H	1:B:386:HIS:CE1	2.33	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:HB2	1:B:232:ARG:HH11	1.80	0.47
1:C:241:ILE:C	1:C:243:ALA:N	2.73	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:A:335:MET:HA	1:A:335:MET:HE2	1.97	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:A:334:ARG:HB3	1:A:335:MET:HE3	1.97	0.46
1:C:55:GLN:HG2	1:D:84:LYS:HE2	1.97	0.46
1:D:331:MET:CE	1:D:331:MET:HA	2.46	0.46
1:B:136:THR:HG22	1:B:138:LEU:H	1.80	0.46
1:D:200:THR:C	1:D:204:LEU:HD12	2.41	0.46
1:B:334:ARG:HH11	1:B:334:ARG:CG	2.29	0.45
1:D:328:HIS:O	1:D:332:VAL:HG23	2.15	0.45
1:A:123:LYS:HB3	1:A:123:LYS:HE2	1.59	0.45
1:B:135:MET:HE3	1:B:335:MET:HE3	1.98	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:C:115:MET:HE2	1:C:314:LEU:HD23	1.97	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:262:GLU:CD	1:B:262:GLU:N	2.75	0.45
1:B:69:GLU:HG3	1:B:143:PHE:CD2	2.52	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:LYS:HE3	1:D:55:GLN:OE1	2.17	0.44
1:B:304:PHE:C	1:B:307:PRO:HD2	2.43	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: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:HH11	1:B:334:ARG:HG2	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:A:223:TRP:CE3	1:A:290:GLN:HG2	2.53	0.43
1:A:380:LYS:H	1:A:380:LYS:HD2	1.82	0.43
1:C:250:LYS:HA	1:C:251:GLU:C	2.44	0.43
1:A:216:GLU:H	1:A:216:GLU:CD	2.27	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:B:136:THR:O	1:B:137:ALA:C	2.61	0.43
1:B:55:GLN:CD	1:B:55:GLN:N	2.77	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:D:326:TYR:HB2	1:D:355:VAL:HG21	2.00	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:C:200:THR:O	1:C:201:LEU:C	2.62	0.42
1:A:327:ASN:HD22	1:A:327:ASN:N	2.17	0.42
1:B:300:GLU:H	1:B:300:GLU:CD	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CBC	2:B:401:HEM:HHD	2.50	0.42
1:C:241:ILE:O	1:C:243:ALA:N	2.53	0.42
1:A:55:GLN:N	1:A:55:GLN:CD	2.78	0.42
1:B:41:ILE:O	1:B:42:TYR:C	2.63	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:C:321:MET:HE3	1:C:321:MET:HB3	1.95	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:C:83:PHE:O	1:C:84:LYS:C	2.63	0.41
1:D:269:ASP:OD2	1:D:272:ARG:HB2	2.20	0.41
1:D:48:LEU:HD23	1:D:48:LEU:HA	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:C:381:MET:HE3	1:C:381:MET:HB2	1.62	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:B:266:SER:CA	1:B:272:ARG:NH2	2.82	0.41
1:C:269:ASP:CG	1:C:272:ARG:HB2	2.45	0.41
1:D:159:ARG:O	1:D:160:LEU:C	2.64	0.40
1:B:165:ILE:HG22	1:B:361:VAL:HG21	2.04	0.40
1:B:360:LYS:O	1:B:363:VAL:HG12	2.21	0.40
1:C:154:GLN:H	1:C:154:GLN:HG2	1.76	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/391 (80%)	296 (94%)	15 (5%)	3 (1%)	12	20
1	B	301/391 (77%)	270 (90%)	24 (8%)	7 (2%)	5	8
1	C	315/391 (81%)	280 (89%)	32 (10%)	3 (1%)	12	20
1	D	283/391 (72%)	247 (87%)	26 (9%)	10 (4%)	3	4
All	All	1213/1564 (78%)	1093 (90%)	97 (8%)	23 (2%)	6	10

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
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 [i](#)

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%)	253 (85%)	44 (15%)	3	4
1	B	287/356 (81%)	242 (84%)	45 (16%)	2	3
1	C	297/356 (83%)	250 (84%)	47 (16%)	2	3
1	D	272/356 (76%)	220 (81%)	52 (19%)	1	2
All	All	1153/1424 (81%)	965 (84%)	188 (16%)	2	3

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	53	ASN
1	A	65	LYS
1	A	84	LYS
1	A	90	LEU
1	A	99	ASN
1	A	102	VAL
1	A	110	LYS
1	A	138	LEU
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	256	GLU
1	A	271	LYS
1	A	289	LEU
1	A	299	ARG
1	A	300	GLU
1	A	303	ARG
1	A	307	PRO

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Mol	Chain	Res	Type
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	356	SER
1	A	358	ARG
1	A	372	LEU
1	A	380	LYS
1	A	381	MET
1	B	62	LYS
1	B	90	LEU
1	B	98	GLN
1	B	115	MET
1	B	119	SER
1	B	123	LYS
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
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	254	VAL
1	B	257	PHE
1	B	259	LYS
1	B	262	GLU
1	B	263	VAL
1	B	265	LEU
1	B	271	LYS

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Mol	Chain	Res	Type
1	B	272	ARG
1	B	274	GLU
1	B	278	SER
1	B	289	LEU
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	381	MET
1	C	41	ILE
1	C	44	ASN
1	C	73	ILE
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
1	C	144	ARG
1	C	147	LEU
1	C	154	GLN
1	C	159	ARG
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	196	GLU
1	C	199	LYS
1	C	211	ARG
1	C	218	HIS
1	C	225	LYS

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Mol	Chain	Res	Type
1	C	228	LYS
1	C	229	ASN
1	C	236	GLU
1	C	256	GLU
1	C	259	LYS
1	C	272	ARG
1	C	274	GLU
1	C	279	LYS
1	C	281	GLU
1	C	282	ARG
1	C	290	GLN
1	C	293	LEU
1	C	296	TYR
1	C	299	ARG
1	C	317	ILE
1	C	319	SER
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	D	41	ILE
1	D	57	LEU
1	D	61	THR
1	D	62	LYS
1	D	66	ILE
1	D	71	LEU
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	123	LYS
1	D	127	GLN
1	D	136	THR
1	D	138	LEU
1	D	141	ASN
1	D	147	LEU
1	D	161	LEU
1	D	164	LYS

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Mol	Chain	Res	Type
1	D	185	LYS
1	D	187	GLU
1	D	188	GLU
1	D	192	LEU
1	D	205	VAL
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	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
1	D	385	ILE
1	D	387	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	70	HIS
1	A	98	GLN
1	A	99	ASN
1	A	107	ASN
1	A	128	GLN

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	242	GLN
1	A	275	HIS
1	A	290	GLN
1	A	305	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	273	HIS
1	B	275	HIS
1	B	327	ASN
1	B	349	HIS
1	B	382	ASN
1	B	386	HIS
1	C	98	GLN
1	C	189	ASN
1	C	197	GLN
1	C	229	ASN
1	C	275	HIS
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	309	GLN
1	D	382	ASN
1	D	386	HIS

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 oligosaccharides 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
4	TRP	A	403	-	14,16,16	2.81	8 (57%)	20,22,22	1.17	2 (10%)
2	HEM	A	401	3,1	50,50,50	1.71	10 (20%)	66,82,82	1.89	18 (27%)
3	9R9	B	402	2	19,19,19	3.33	7 (36%)	21,28,28	2.43	6 (28%)
2	HEM	C	401	3,1	50,50,50	1.67	9 (18%)	66,82,82	1.91	15 (22%)
2	HEM	D	401	3,1	50,50,50	1.61	9 (18%)	66,82,82	1.77	16 (24%)
4	TRP	B	403	-	14,16,16	2.57	4 (28%)	20,22,22	1.13	2 (10%)
4	TRP	D	403	-	14,16,16	2.74	6 (42%)	20,22,22	1.31	3 (15%)
5	CIT	A	404	-	12,12,12	1.27	0	17,17,17	1.79	5 (29%)
3	9R9	D	402	2	19,19,19	2.71	8 (42%)	21,28,28	3.78	12 (57%)
3	9R9	A	402	2	19,19,19	2.58	7 (36%)	21,28,28	1.83	5 (23%)
2	HEM	B	401	3,1	50,50,50	1.56	11 (22%)	66,82,82	1.96	20 (30%)
3	9R9	C	402	2	19,19,19	3.08	9 (47%)	21,28,28	2.31	6 (28%)

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
4	TRP	A	403	-	-	2/8/8/8	0/2/2/2
2	HEM	A	401	3,1	-	8/14/54/54	-
3	9R9	B	402	2	-	0/6/16/16	0/3/3/3
2	HEM	C	401	3,1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	401	3,1	-	8/14/54/54	-
4	TRP	B	403	-	-	2/8/8/8	0/2/2/2
4	TRP	D	403	-	-	2/8/8/8	0/2/2/2
5	CIT	A	404	-	-	9/16/16/16	-
3	9R9	D	402	2	-	0/6/16/16	0/3/3/3
3	9R9	A	402	2	-	0/6/16/16	0/3/3/3
2	HEM	B	401	3,1	-	2/14/54/54	-
3	9R9	C	402	2	-	0/6/16/16	0/3/3/3

All (88) 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	CAE-CAI	-6.25	1.34	1.42
4	D	403	TRP	CD2-CG	-6.24	1.33	1.44
3	C	402	9R9	CAE-CAI	-5.58	1.35	1.42
3	D	402	9R9	CAE-CAI	-5.33	1.35	1.42
4	B	403	TRP	CD2-CG	-5.28	1.35	1.44
4	A	403	TRP	CD2-CE2	-5.28	1.34	1.41
3	A	402	9R9	CAJ-CAF	-5.22	1.47	1.53
2	A	401	HEM	FE-NB	5.16	2.10	1.94
2	D	401	HEM	FE-NB	5.12	2.10	1.94
4	A	403	TRP	CD2-CG	-5.08	1.35	1.44
3	C	402	9R9	CAE-CAD	-5.07	1.35	1.41
3	D	402	9R9	CAB-CLA	-4.86	1.63	1.74
2	C	401	HEM	C1B-NB	-4.77	1.32	1.40
3	B	402	9R9	CAB-CLA	-4.72	1.64	1.74
2	C	401	HEM	FE-NB	4.65	2.09	1.94
3	D	402	9R9	NAG-NAH	-4.58	1.33	1.36
4	D	403	TRP	CD2-CE2	-4.56	1.35	1.41
3	C	402	9R9	CAK-CAJ	4.49	1.59	1.53
3	A	402	9R9	CAE-CAI	-4.49	1.36	1.42
3	B	402	9R9	CAC-CAD	-4.41	1.32	1.39
4	B	403	TRP	CD2-CE2	-4.41	1.35	1.41
2	B	401	HEM	FE-NB	4.35	2.08	1.94
2	A	401	HEM	C1B-NB	-4.25	1.33	1.40
2	C	401	HEM	C1C-C2C	-4.25	1.36	1.45
2	A	401	HEM	FE-NC	4.19	2.09	1.95
3	A	402	9R9	CAB-CLA	-4.17	1.65	1.74
4	B	403	TRP	CB-CG	4.14	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	9R9	CAC-CAD	-4.13	1.33	1.39
2	D	401	HEM	C1B-NB	-4.10	1.33	1.40
3	D	402	9R9	CAK-CAJ	-4.00	1.48	1.53
3	C	402	9R9	CAC-CAD	-3.93	1.33	1.39
3	A	402	9R9	CAE-CAD	-3.83	1.37	1.41
3	B	402	9R9	CAE-CAD	-3.82	1.37	1.41
2	A	401	HEM	C4D-C3D	3.82	1.51	1.45
3	B	402	9R9	CAE-CAF	-3.69	1.36	1.42
3	D	402	9R9	CAE-CAD	-3.68	1.37	1.41
3	C	402	9R9	NAG-NAH	-3.61	1.34	1.36
4	A	403	TRP	CE3-CD2	-3.58	1.34	1.39
4	D	403	TRP	CZ2-CE2	-3.50	1.33	1.39
3	D	402	9R9	CAC-CAD	-3.42	1.34	1.39
2	A	401	HEM	C4D-ND	-3.32	1.34	1.40
4	A	403	TRP	CZ2-CE2	-3.22	1.34	1.39
4	D	403	TRP	CE3-CD2	-3.21	1.34	1.39
2	C	401	HEM	FE-NC	3.09	2.05	1.95
2	B	401	HEM	C4D-ND	-3.09	1.35	1.40
4	A	403	TRP	CB-CG	3.09	1.56	1.50
3	A	402	9R9	NAG-NAH	-3.02	1.34	1.36
2	C	401	HEM	C4C-NC	-3.01	1.33	1.39
4	A	403	TRP	CE2-NE1	-2.94	1.32	1.37
2	D	401	HEM	FE-NC	2.87	2.04	1.95
2	B	401	HEM	C4D-C3D	2.83	1.49	1.45
2	B	401	HEM	FE-NC	2.80	2.04	1.95
2	B	401	HEM	C1B-NB	-2.80	1.35	1.40
3	C	402	9R9	CAE-CAF	-2.79	1.38	1.42
4	A	403	TRP	CD1-NE1	-2.77	1.32	1.37
2	C	401	HEM	C1D-ND	-2.73	1.33	1.38
2	B	401	HEM	C1D-C2D	2.71	1.49	1.44
2	D	401	HEM	C4B-NB	-2.65	1.33	1.38
2	B	401	HEM	C3B-C4B	2.64	1.50	1.44
4	B	403	TRP	CE3-CD2	-2.64	1.35	1.39
2	B	401	HEM	C1C-NC	-2.61	1.34	1.39
2	C	401	HEM	C4D-ND	-2.55	1.35	1.40
2	A	401	HEM	C1D-C2D	2.55	1.49	1.44
4	D	403	TRP	CE2-NE1	-2.53	1.33	1.37
2	B	401	HEM	C4B-NB	-2.53	1.33	1.38
2	A	401	HEM	C3B-C4B	2.53	1.49	1.44
3	D	402	9R9	CAI-NAH	2.49	1.33	1.32
3	B	402	9R9	CAK-CAJ	2.47	1.56	1.53
2	D	401	HEM	C3B-C4B	2.46	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	9R9	CAB-CLA	-2.41	1.69	1.74
2	A	401	HEM	C3C-C2C	2.29	1.41	1.37
4	D	403	TRP	CB-CG	2.28	1.54	1.50
2	D	401	HEM	C3C-C4C	-2.27	1.42	1.46
2	D	401	HEM	C1B-C2B	-2.24	1.40	1.44
2	D	401	HEM	O1A-CGA	2.23	1.29	1.22
4	A	403	TRP	CD1-CG	-2.22	1.33	1.36
2	B	401	HEM	C3C-C4C	-2.15	1.42	1.46
2	D	401	HEM	C1D-ND	-2.11	1.34	1.38
2	A	401	HEM	C4C-NC	-2.11	1.35	1.39
3	A	402	9R9	CAE-CAF	-2.06	1.39	1.42
2	C	401	HEM	C4B-NB	-2.06	1.34	1.38
2	C	401	HEM	CHD-C4C	-2.06	1.34	1.38
3	C	402	9R9	CAK-CAL	2.04	1.57	1.52
2	A	401	HEM	O2A-CGA	-2.03	1.23	1.30
3	D	402	9R9	CAJ-CAF	-2.02	1.51	1.53
2	B	401	HEM	O1D-CGD	2.00	1.28	1.22

All (110) 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	B	402	9R9	CAE-CAI-NAH	-7.48	109.03	111.41
3	D	402	9R9	CAO-CAJ-CAK	6.91	118.18	108.80
3	C	402	9R9	CAL-CAK-CAJ	6.14	116.02	112.60
3	D	402	9R9	OAP-CAJ-CAK	5.87	121.00	107.69
2	D	401	HEM	C1B-NB-C4B	5.39	110.64	105.07
2	C	401	HEM	C1B-NB-C4B	5.25	110.49	105.07
3	A	402	9R9	CAE-CAI-NAH	-5.18	109.76	111.41
3	B	402	9R9	CAL-CAK-CAJ	5.10	115.44	112.60
2	B	401	HEM	C1B-NB-C4B	5.03	110.27	105.07
2	C	401	HEM	CHC-C4B-NB	4.92	129.76	124.42
3	D	402	9R9	CAL-CAK-CAJ	-4.85	109.89	112.60
2	C	401	HEM	C4C-NC-C1C	4.83	110.08	105.35
2	B	401	HEM	CAD-CBD-CGD	4.66	123.64	113.60
2	B	401	HEM	CBD-CAD-C3D	-4.61	99.81	112.63
2	A	401	HEM	CAD-CBD-CGD	4.52	123.33	113.60
3	D	402	9R9	OAP-CAJ-CAO	4.37	117.60	107.69
3	C	402	9R9	CAE-CAI-NAH	-4.32	110.03	111.41
2	C	401	HEM	CHC-C1C-NC	4.21	129.00	124.44
2	C	401	HEM	CBD-CAD-C3D	-4.09	101.26	112.63
2	A	401	HEM	CBD-CAD-C3D	-4.00	101.51	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	CHD-C4C-NC	3.99	128.76	124.44
2	A	401	HEM	O2D-CGD-CBD	3.94	126.69	114.03
3	D	402	9R9	CAE-CAD-NAG	3.93	109.65	106.47
2	B	401	HEM	C2D-C1D-ND	3.93	114.59	109.88
2	A	401	HEM	CHD-C1D-C2D	-3.93	118.84	124.98
2	D	401	HEM	C4C-NC-C1C	3.85	109.12	105.35
2	D	401	HEM	CHD-C1D-C2D	-3.84	118.97	124.98
2	D	401	HEM	CHD-C4C-NC	3.77	128.52	124.44
2	B	401	HEM	C4C-NC-C1C	3.76	109.03	105.35
3	B	402	9R9	CAI-NAH-NAG	3.70	107.98	106.02
2	C	401	HEM	CHA-C4D-ND	3.67	128.89	124.37
5	A	404	CIT	C3-C4-C5	3.52	122.33	113.81
2	C	401	HEM	CHD-C1D-ND	3.51	128.23	124.42
3	C	402	9R9	CAE-CAD-NAG	3.51	109.31	106.47
3	C	402	9R9	CAI-NAH-NAG	3.35	107.79	106.02
2	A	401	HEM	O2D-CGD-O1D	-3.31	115.05	123.30
2	D	401	HEM	CAD-CBD-CGD	3.24	120.58	113.60
2	A	401	HEM	C1D-C2D-C3D	-3.22	103.57	106.96
2	B	401	HEM	C1D-C2D-C3D	-3.17	103.62	106.96
2	B	401	HEM	CHD-C1D-C2D	-3.14	120.07	124.98
2	C	401	HEM	CHD-C1D-C2D	-3.07	120.18	124.98
3	C	402	9R9	CAO-CAJ-CAK	3.07	112.97	108.80
2	A	401	HEM	CHD-C1D-ND	3.07	127.75	124.42
5	A	404	CIT	O6-C6-C3	3.07	118.37	113.05
2	B	401	HEM	CMD-C2D-C1D	3.06	129.70	125.04
2	D	401	HEM	CHD-C1D-ND	3.03	127.71	124.42
2	A	401	HEM	C4C-NC-C1C	3.00	108.28	105.35
2	D	401	HEM	CHA-C4D-ND	2.98	128.04	124.37
3	A	402	9R9	CAI-NAH-NAG	2.94	107.58	106.02
2	A	401	HEM	C2D-C1D-ND	2.94	113.40	109.88
2	A	401	HEM	CMD-C2D-C1D	2.89	129.43	125.04
2	A	401	HEM	C1B-NB-C4B	2.87	108.04	105.07
4	A	403	TRP	CG-CD1-NE1	-2.85	107.00	110.31
2	C	401	HEM	C1A-CHA-C4D	-2.85	119.59	126.34
2	A	401	HEM	CHC-C4B-NB	2.85	127.51	124.42
2	D	401	HEM	C2D-C1D-ND	2.83	113.28	109.88
2	B	401	HEM	CAD-C3D-C4D	2.83	129.60	124.66
2	D	401	HEM	CHB-C1B-NB	2.79	127.82	124.37
5	A	404	CIT	C2-C3-C6	-2.73	104.23	110.11
2	B	401	HEM	C3D-C4D-ND	2.68	113.15	110.17
3	D	402	9R9	CAN-CAO-CAJ	-2.66	111.12	112.60
4	D	403	TRP	CD2-CG-CD1	2.65	109.02	106.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CHA-C4D-C3D	-2.63	120.40	125.33
3	D	402	9R9	CAB-CAA-CAF	2.62	122.00	118.39
4	B	403	TRP	CD2-CG-CD1	2.60	108.96	106.15
2	D	401	HEM	C1A-CHA-C4D	-2.56	120.26	126.34
3	A	402	9R9	CAE-CAD-NAG	2.56	108.54	106.47
2	B	401	HEM	CHC-C4B-NB	2.55	127.19	124.42
2	A	401	HEM	CAD-C3D-C4D	2.55	129.12	124.66
2	B	401	HEM	CHA-C1A-NA	2.55	128.54	123.85
3	A	402	9R9	CAO-CAJ-CAK	2.53	112.24	108.80
2	B	401	HEM	C4D-ND-C1D	-2.53	102.46	105.07
3	D	402	9R9	CAI-NAH-NAG	2.53	107.36	106.02
2	C	401	HEM	C4B-C3B-C2B	-2.52	105.11	107.11
4	B	403	TRP	CG-CD1-NE1	-2.49	107.42	110.31
4	D	403	TRP	CE3-CD2-CE2	2.48	121.49	118.83
2	B	401	HEM	O2D-CGD-CBD	2.47	121.96	114.03
3	D	402	9R9	CAA-CAF-CAE	-2.46	114.77	117.63
2	C	401	HEM	C1C-CHC-C4B	-2.43	120.81	126.06
2	B	401	HEM	CHB-C1B-NB	2.42	127.36	124.37
4	A	403	TRP	CD2-CG-CD1	2.37	108.72	106.15
5	A	404	CIT	O5-C6-C3	-2.35	118.93	122.25
2	C	401	HEM	CHA-C4D-C3D	-2.32	120.97	125.33
2	C	401	HEM	CMD-C2D-C1D	2.29	128.52	125.04
2	D	401	HEM	O2D-CGD-CBD	2.28	121.36	114.03
3	B	402	9R9	CAE-CAD-NAG	2.27	108.31	106.47
2	B	401	HEM	CHA-C4D-C3D	-2.26	121.09	125.33
3	A	402	9R9	CAC-CAB-CLA	-2.25	116.34	119.15
2	A	401	HEM	CHB-C4A-C3A	-2.24	120.90	127.24
2	D	401	HEM	CHC-C4B-NB	2.24	126.85	124.42
3	D	402	9R9	CAC-CAD-NAG	-2.23	128.54	132.31
2	A	401	HEM	CAD-C3D-C2D	-2.22	123.74	127.88
2	C	401	HEM	O2A-CGA-CBA	2.20	121.11	114.03
3	D	402	9R9	CAF-CAE-CAI	2.19	133.56	125.81
4	D	403	TRP	CG-CD1-NE1	-2.18	107.78	110.31
2	D	401	HEM	CMD-C2D-C3D	2.17	132.02	126.12
2	B	401	HEM	CMC-C2C-C1C	2.16	128.52	124.71
3	B	402	9R9	CAN-CAO-CAJ	-2.14	111.40	112.60
2	A	401	HEM	CHB-C4A-NA	2.13	127.77	123.85
2	D	401	HEM	C4C-CHD-C1D	-2.10	121.53	126.06
2	A	401	HEM	CAA-C2A-C3A	-2.09	122.28	127.07
3	C	402	9R9	OAP-CAJ-CAK	-2.05	103.04	107.69
2	B	401	HEM	C1A-CHA-C4D	-2.05	121.48	126.34
5	A	404	CIT	O1-C1-C2	-2.05	116.96	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	CHD-C4C-C3C	-2.05	121.76	125.26
3	B	402	9R9	CAO-CAJ-CAK	2.03	111.56	108.80
2	B	401	HEM	CAD-C3D-C2D	-2.03	124.10	127.88
2	A	401	HEM	CAA-C2A-C1A	2.02	128.87	124.89
2	C	401	HEM	CAD-C3D-C4D	2.02	128.18	124.66

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	HEM	C2B-C3B-CAB-CBB
2	B	401	HEM	C4B-C3B-CAB-CBB
5	A	404	CIT	C2-C3-C4-C5
5	A	404	CIT	C6-C3-C4-C5
2	D	401	HEM	C3D-CAD-CBD-CGD
5	A	404	CIT	C1-C2-C3-C4
5	A	404	CIT	C1-C2-C3-C6
2	D	401	HEM	C2C-C3C-CAC-CBC
5	A	404	CIT	O7-C3-C4-C5
2	D	401	HEM	C4C-C3C-CAC-CBC
4	A	403	TRP	CA-CB-CG-CD2
2	A	401	HEM	C1A-C2A-CAA-CBA
5	A	404	CIT	C2-C3-C6-O5
5	A	404	CIT	C4-C3-C6-O5
4	D	403	TRP	CA-CB-CG-CD2
4	A	403	TRP	CA-CB-CG-CD1
4	D	403	TRP	CA-CB-CG-CD1
5	A	404	CIT	C2-C3-C6-O6
5	A	404	CIT	C4-C3-C6-O6
2	A	401	HEM	C3A-C2A-CAA-CBA
2	A	401	HEM	C2C-C3C-CAC-CBC
2	D	401	HEM	C2A-CAA-CBA-CGA
2	A	401	HEM	C4C-C3C-CAC-CBC
4	B	403	TRP	CA-CB-CG-CD2
2	D	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	C4D-C3D-CAD-CBD
2	A	401	HEM	CAD-CBD-CGD-O1D

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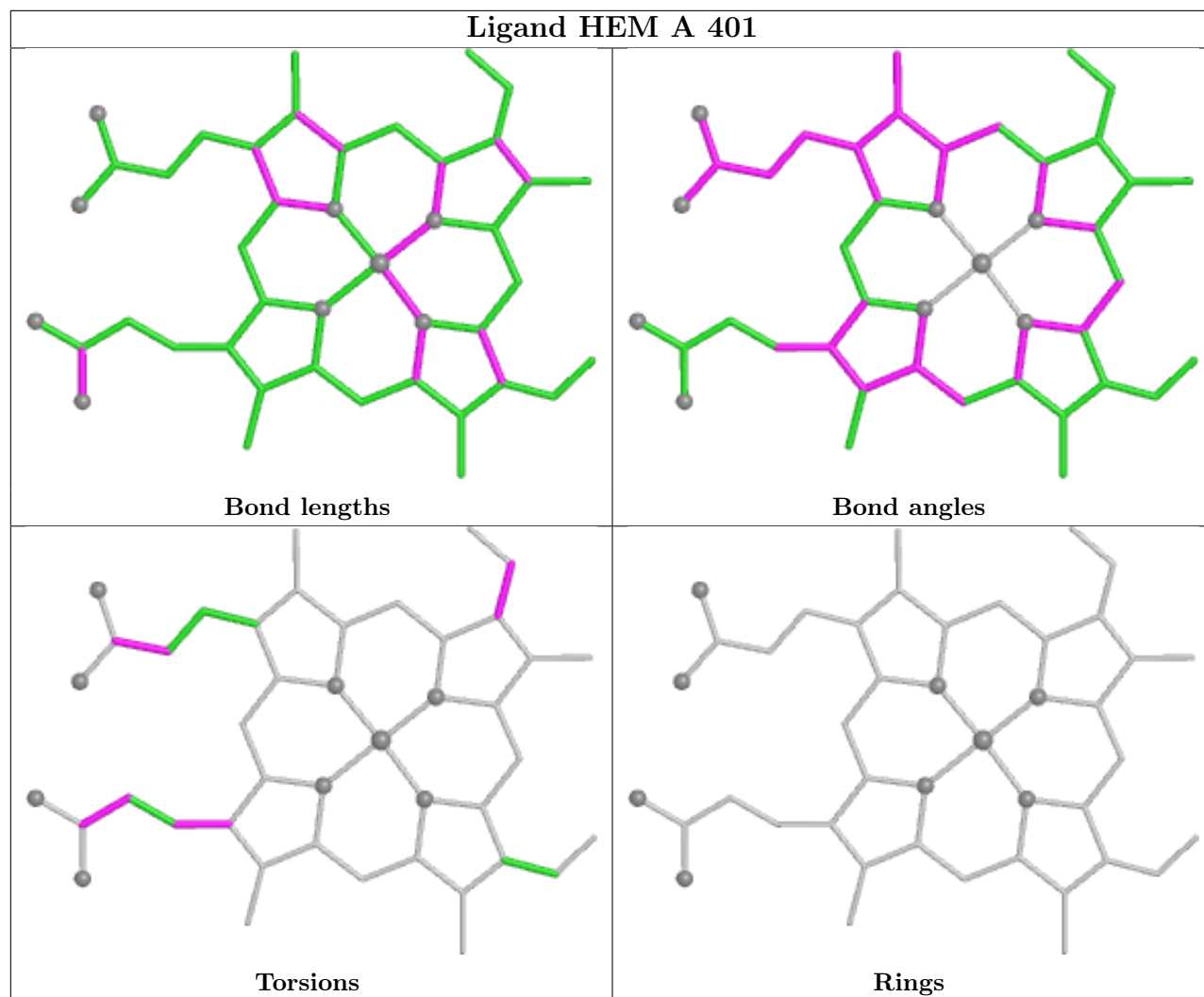
Mol	Chain	Res	Type	Atoms
2	A	401	HEM	CAD-CBD-CGD-O2D
4	B	403	TRP	CA-CB-CG-CD1
2	D	401	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

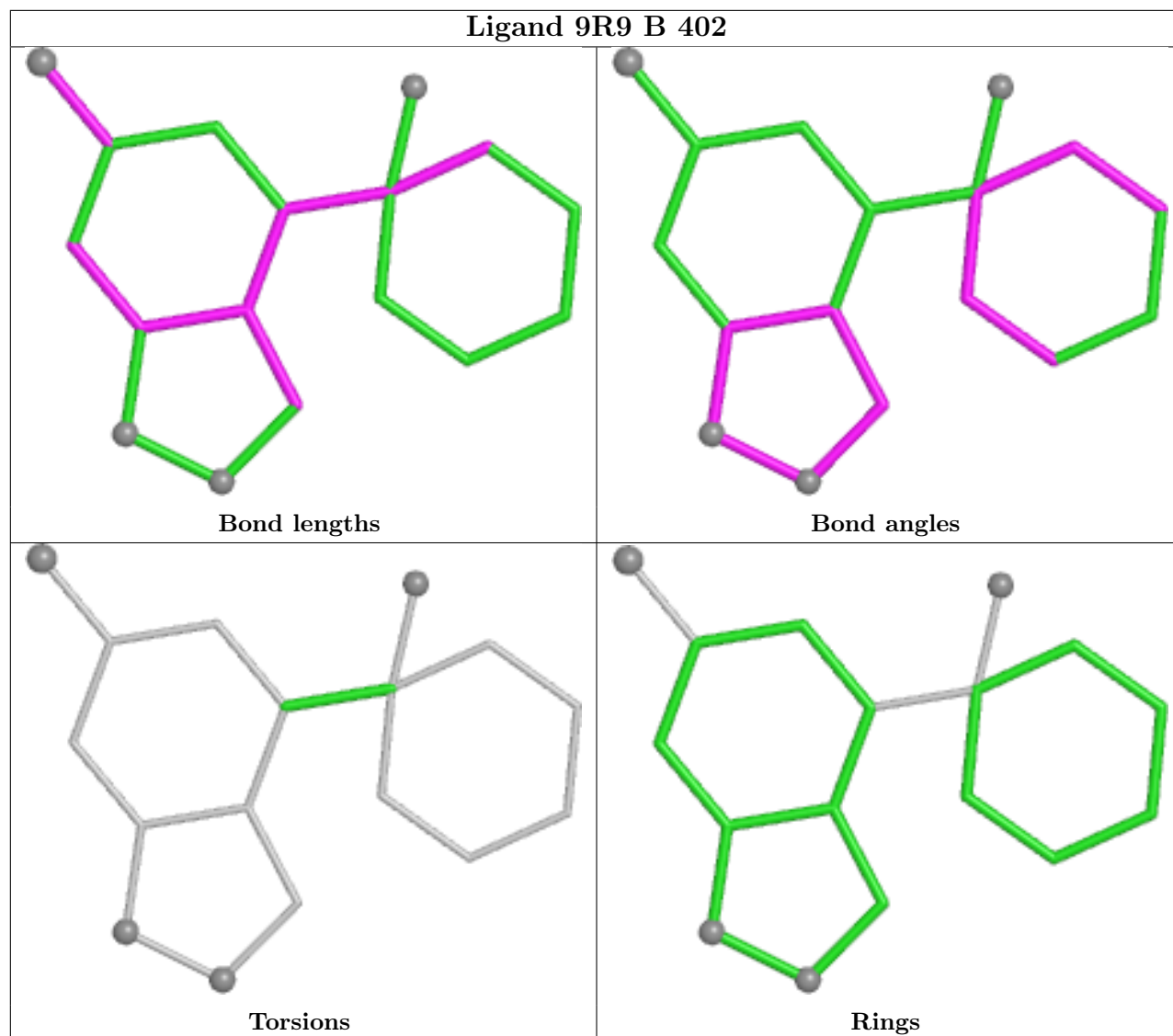
4 monomers are involved in 16 short contacts:

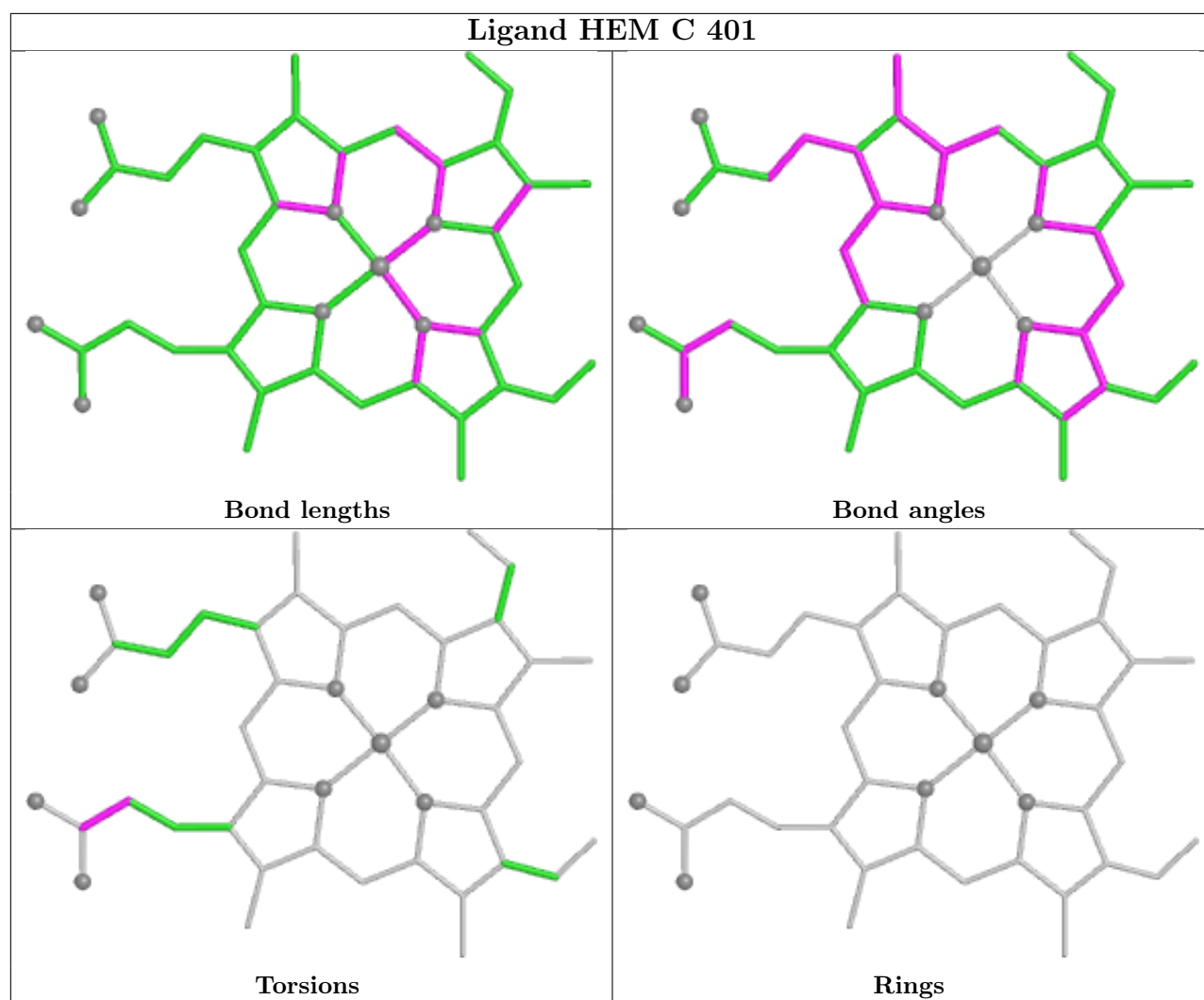
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	4	0
2	C	401	HEM	2	0
2	D	401	HEM	2	0
2	B	401	HEM	8	0

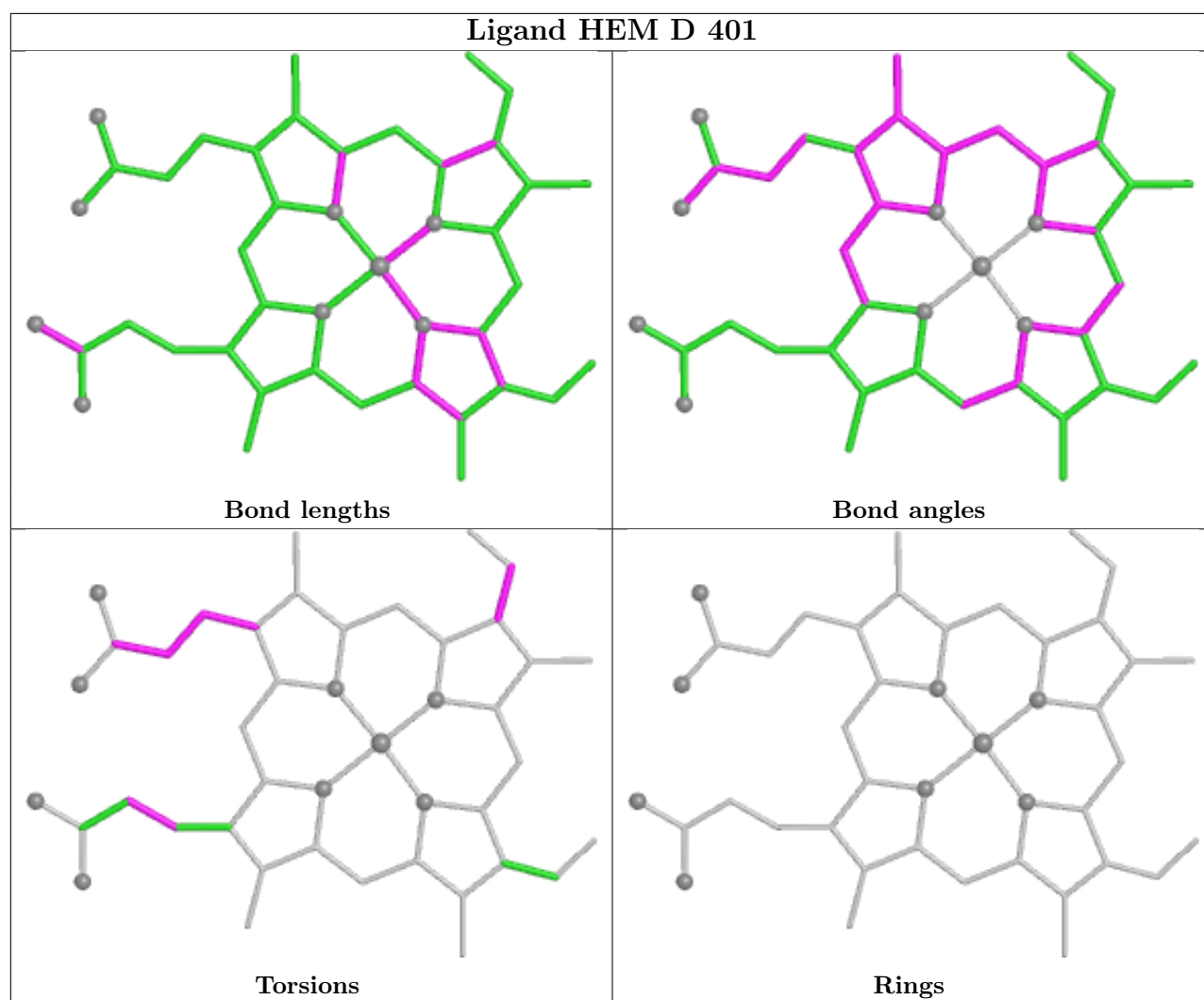
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



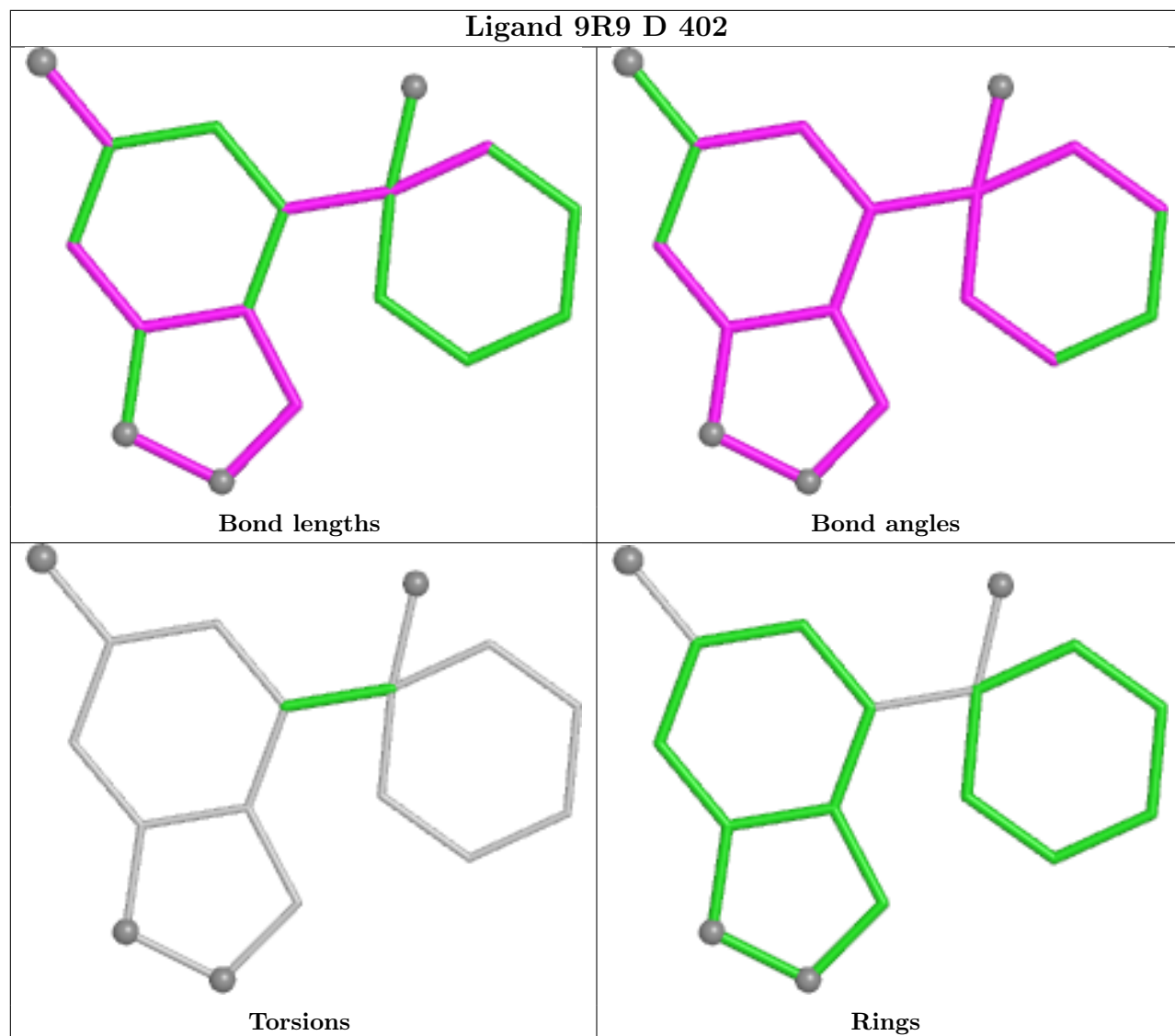
Ligand 9R9 B 402



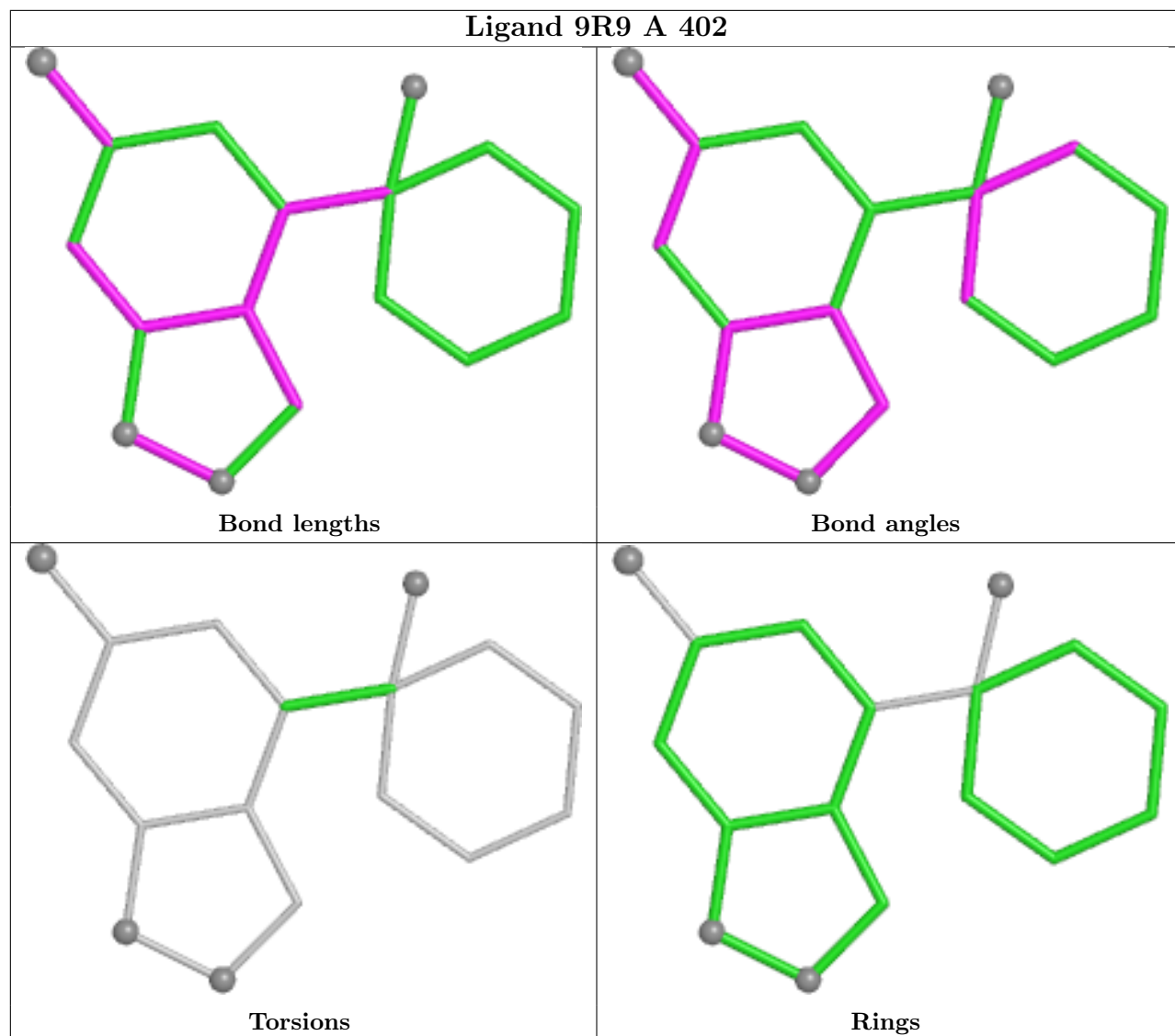


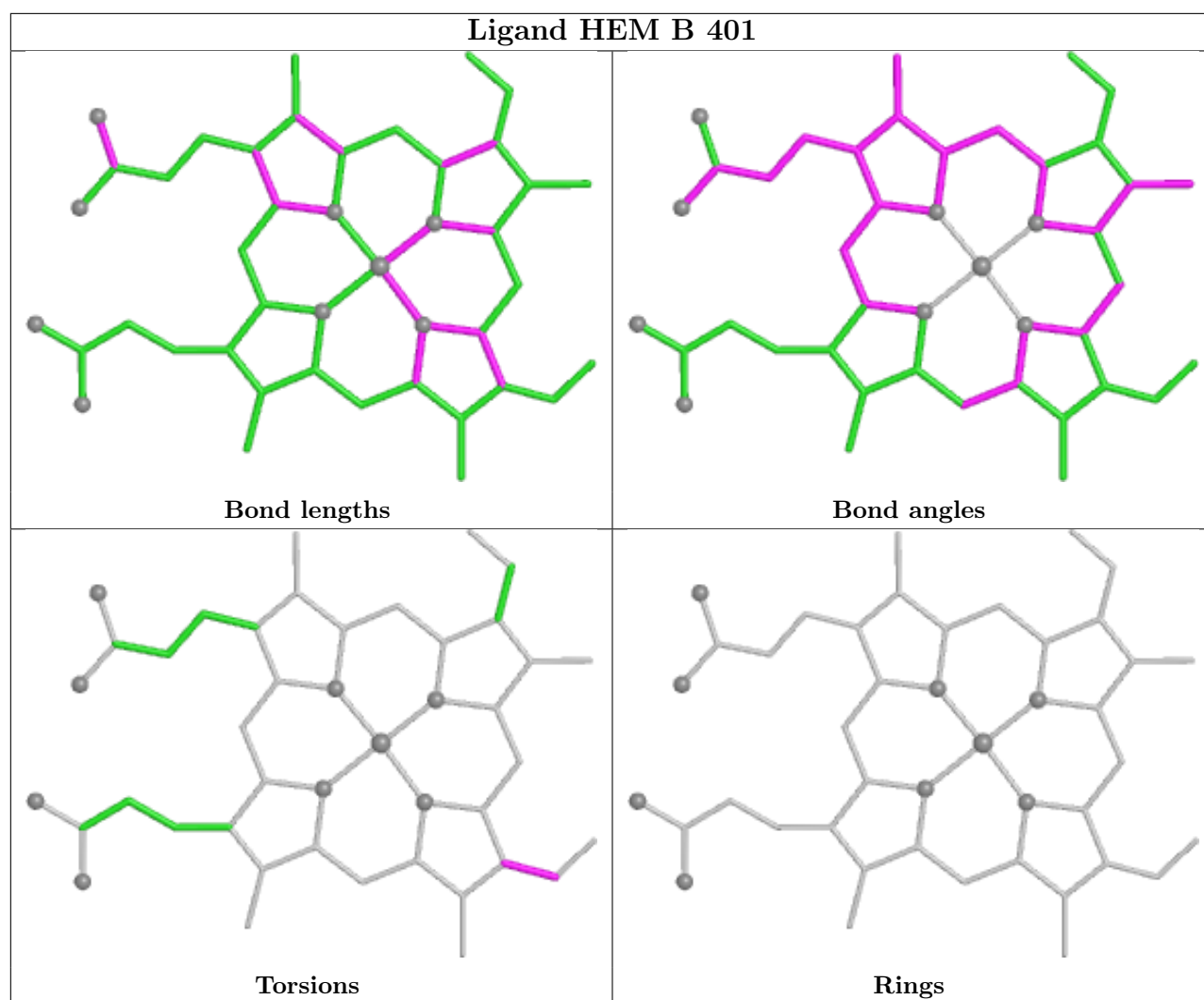


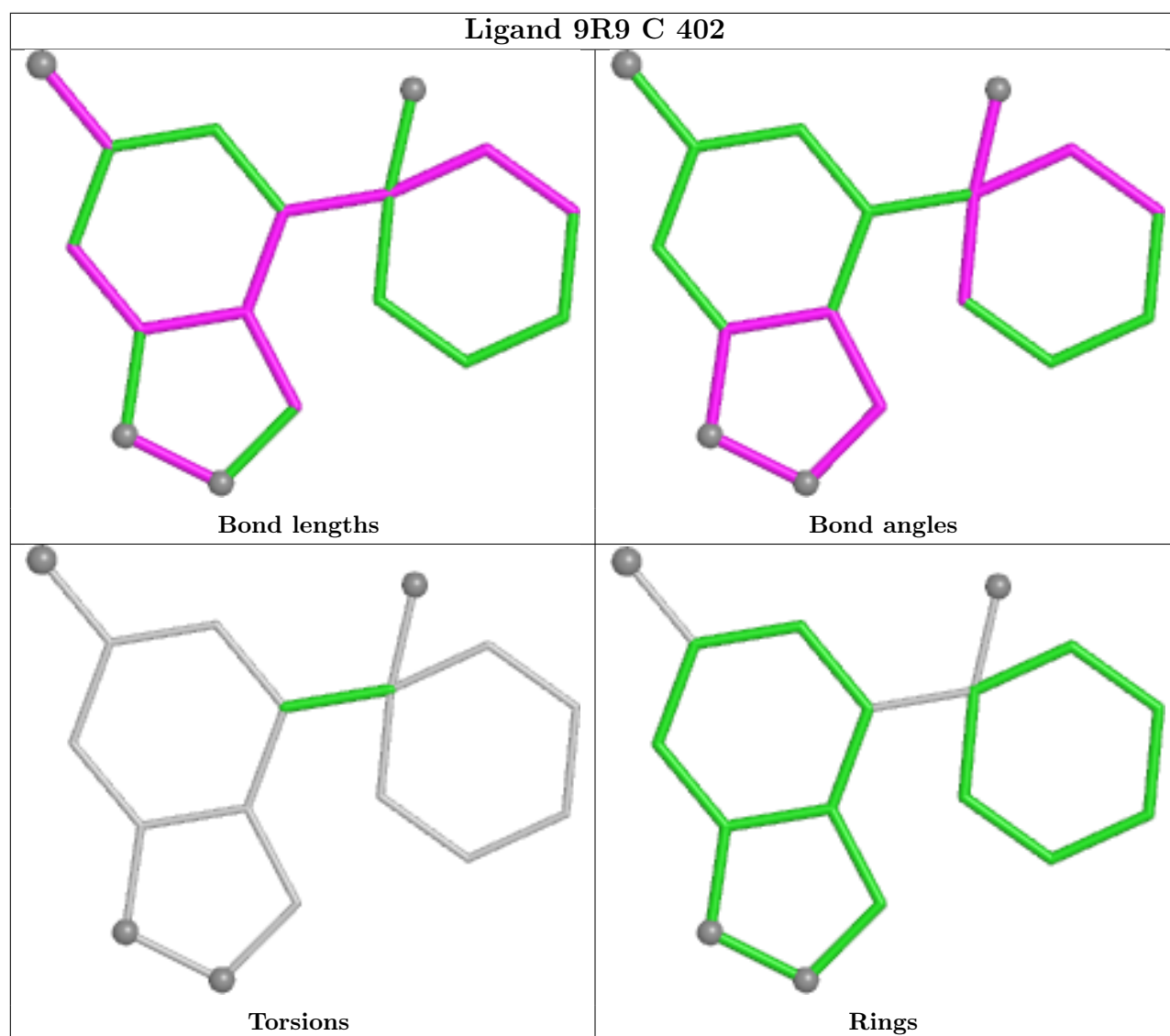
Ligand 9R9 D 402



Ligand 9R9 A 402







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%)	-0.08	13 (4%)	42	34	47, 68, 118, 168	0
1	B	309/391 (79%)	0.06	11 (3%)	46	38	50, 84, 139, 190	0
1	C	323/391 (82%)	0.23	17 (5%)	32	25	58, 97, 146, 170	0
1	D	290/391 (74%)	0.34	29 (10%)	12	10	55, 97, 148, 169	1 (0%)
All	All	1244/1564 (79%)	0.13	70 (5%)	30	24	47, 86, 144, 190	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ALA	6.4
1	D	264	LEU	5.7
1	D	40	LEU	4.7
1	A	248	GLU	4.6
1	D	375[A]	ARG	4.5
1	A	344	GLY	4.3
1	C	41	ILE	4.1
1	B	385	ILE	3.7
1	B	238	PHE	3.7
1	C	333	HIS	3.6
1	C	185	LYS	3.5
1	D	387	LYS	3.5
1	A	249	GLU	3.5
1	A	170	ASN	3.5
1	C	346	SER	3.3
1	D	224	GLY	3.3
1	C	338	SER	3.2
1	D	185	LYS	3.2
1	D	371	TYR	3.2
1	B	253	GLN	3.0
1	C	250	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	367	ASN	3.0
1	D	262	GLU	3.0
1	C	304	PHE	3.0
1	B	40	LEU	2.9
1	D	334	ARG	2.9
1	C	239	ILE	2.9
1	D	265	LEU	2.9
1	D	135	MET	2.8
1	D	383	PRO	2.8
1	B	351	LEU	2.8
1	C	220	PHE	2.8
1	B	168	LEU	2.7
1	B	257	PHE	2.7
1	A	338	SER	2.7
1	D	263	VAL	2.7
1	D	268	PHE	2.7
1	D	192	LEU	2.6
1	A	350	TYR	2.5
1	D	384	THR	2.5
1	D	138	LEU	2.5
1	A	318	ASP	2.5
1	C	173	VAL	2.5
1	D	225	LYS	2.4
1	B	254	VAL	2.4
1	B	371	TYR	2.4
1	C	351	LEU	2.4
1	C	349	HIS	2.4
1	D	348	TYR	2.3
1	D	339	LYS	2.3
1	B	296	TYR	2.3
1	A	366	PHE	2.3
1	B	191	LEU	2.3
1	A	371	TYR	2.3
1	A	250	LYS	2.2
1	D	227	GLU	2.2
1	D	66	ILE	2.2
1	C	251	GLU	2.2
1	C	371	TYR	2.2
1	D	190	GLU	2.2
1	D	193	LEU	2.2
1	D	226	LEU	2.2
1	A	334	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	370	THR	2.1
1	D	386	HIS	2.1
1	C	103	ARG	2.1
1	C	51	VAL	2.0
1	C	178	ARG	2.0
1	D	272	ARG	2.0
1	D	381	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

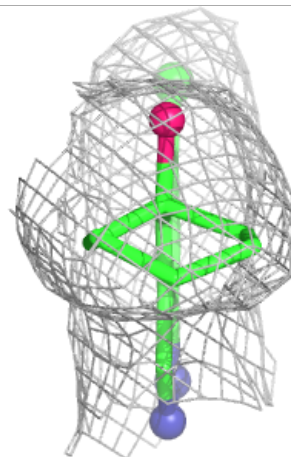
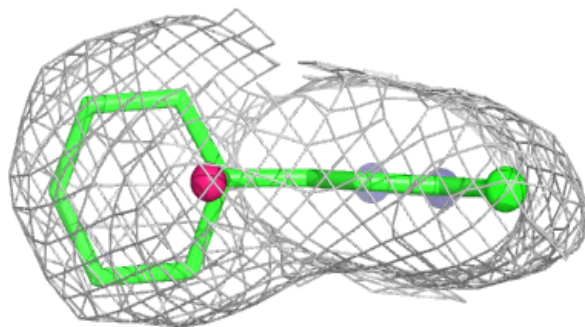
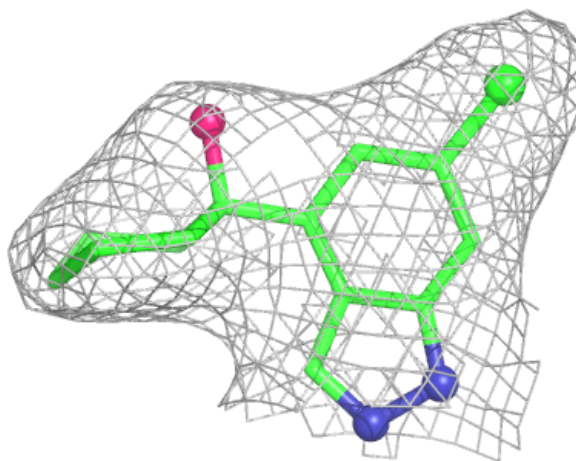
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CIT	A	404	13/13	0.78	0.14	90,121,135,140	0
4	TRP	D	403	15/15	0.93	0.11	83,90,109,117	0
3	9R9	C	402	17/17	0.95	0.07	61,69,78,92	0
4	TRP	B	403	15/15	0.95	0.08	56,66,76,83	0
3	9R9	B	402	17/17	0.96	0.08	63,66,70,82	0
3	9R9	A	402	17/17	0.96	0.08	49,53,69,70	0
3	9R9	D	402	17/17	0.96	0.07	69,74,84,91	0
4	TRP	A	403	15/15	0.97	0.06	52,57,68,72	0
2	HEM	B	401	43/43	0.97	0.08	68,76,98,107	0
2	HEM	C	401	43/43	0.98	0.07	70,80,105,111	0
2	HEM	D	401	43/43	0.98	0.09	78,88,107,109	0
2	HEM	A	401	43/43	0.99	0.06	51,61,82,92	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.

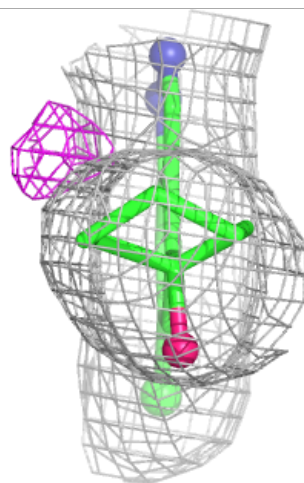
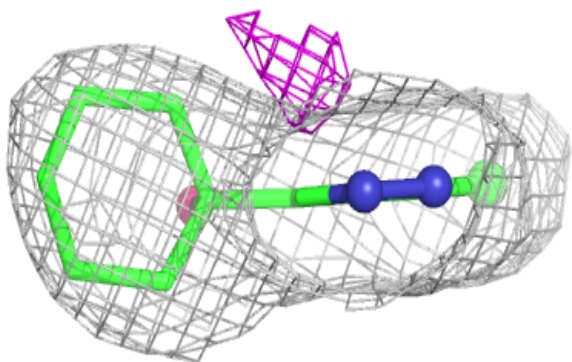
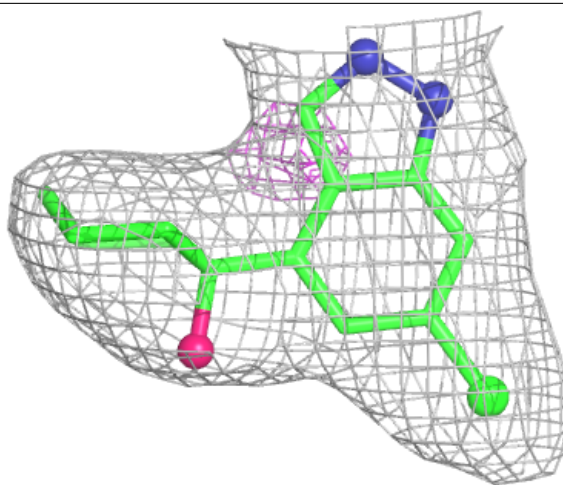
Electron density around 9R9 C 402:

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



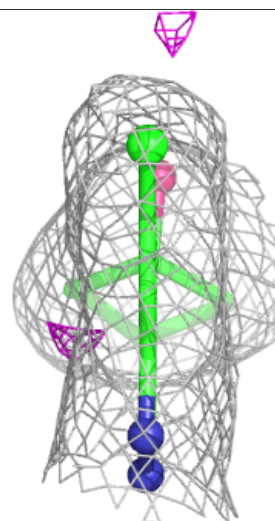
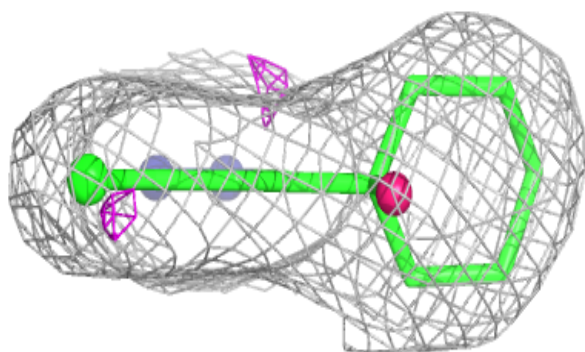
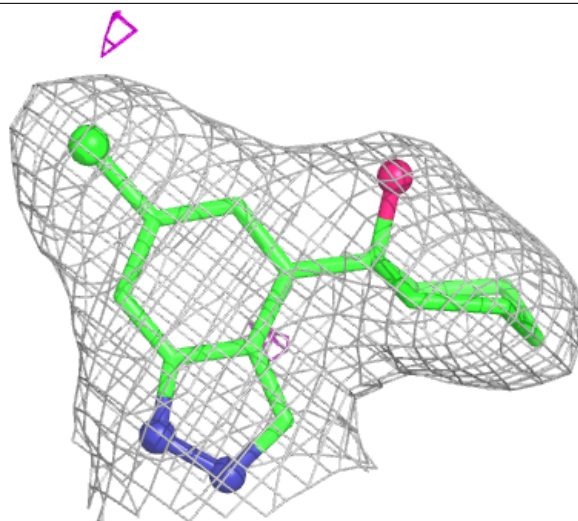
Electron density around 9R9 B 402:

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



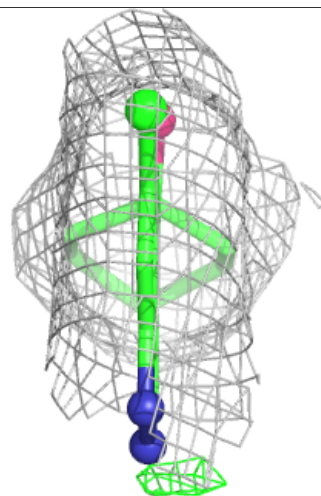
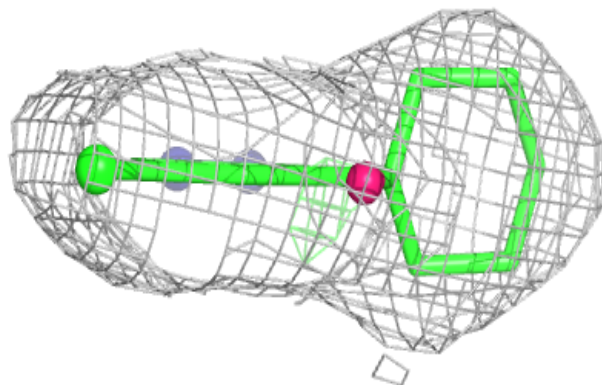
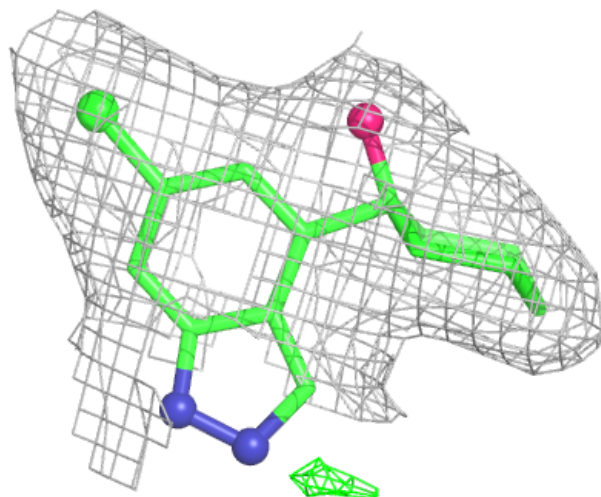
Electron density around 9R9 A 402:

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



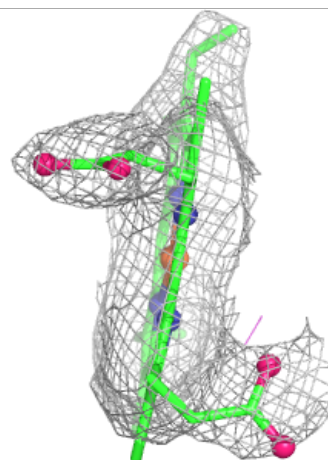
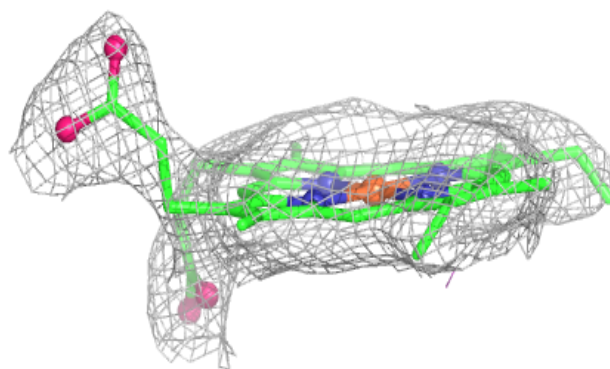
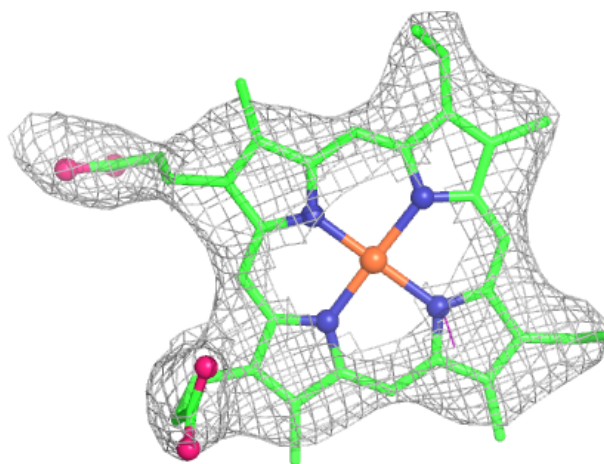
Electron density around 9R9 D 402:

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



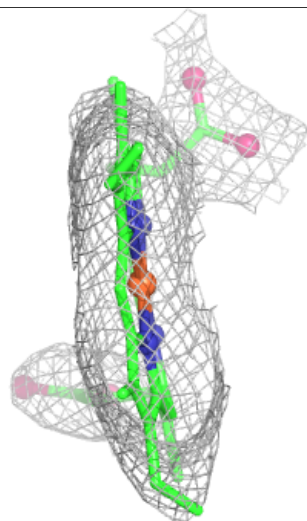
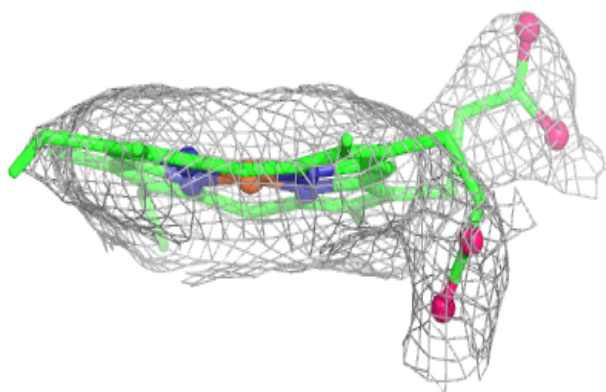
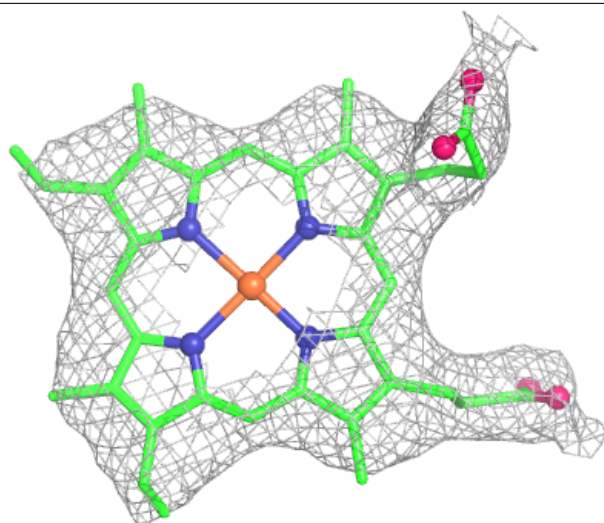
Electron density around HEM B 401:

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



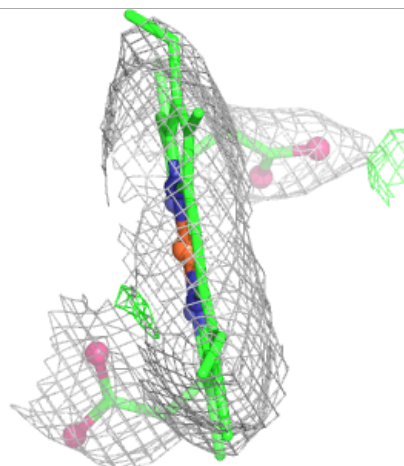
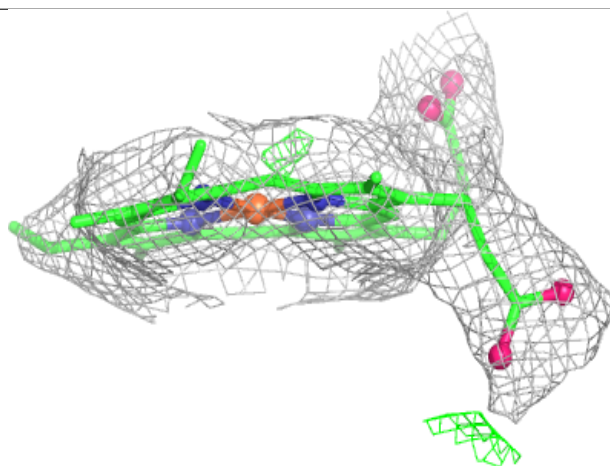
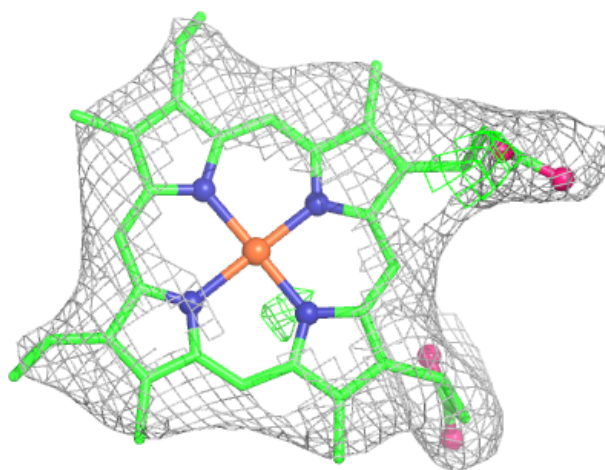
Electron density around HEM C 401:

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



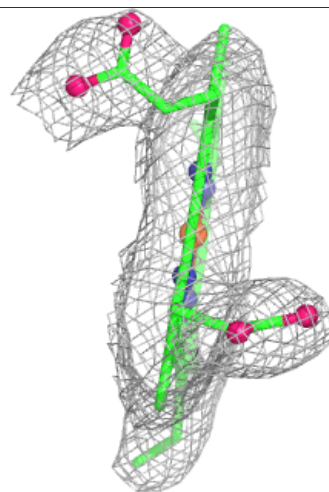
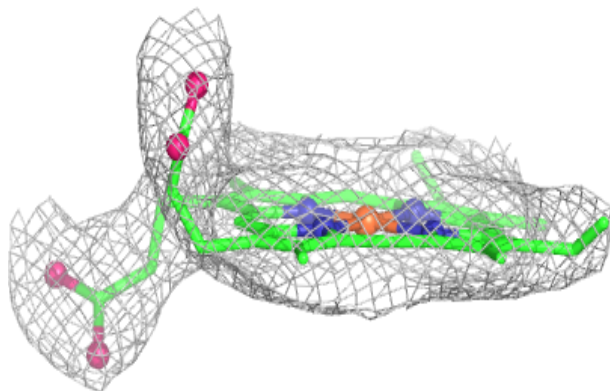
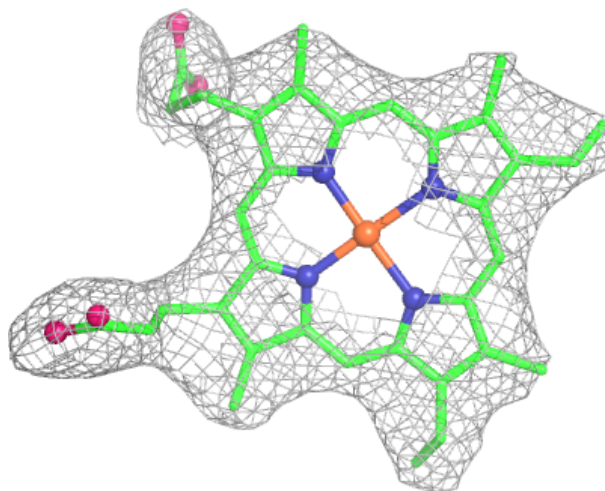
Electron density around HEM D 401:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.