



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:05 PM UTC

PDB ID : 7P0N / pdb_00007p0n
Title : Crystal structure of L-Trp/Indoleamine 2,3-dioxygenase 1 (hIDO1) complex with the JK-loop refined in the open conformation
Authors : Mirgaux, M.; Wouters, J.
Deposited on : 2021-06-30
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

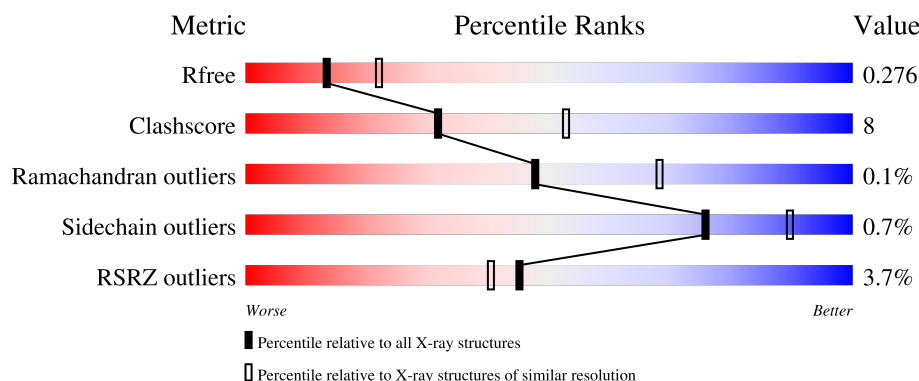
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	405	
1	B	405	
1	C	405	
1	D	405	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	TRP	C	503	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12712 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2924	1880	499	528	17			
1	B	375	Total	C	N	O	S	0	0	0
			2954	1896	504	537	17			
1	C	374	Total	C	N	O	S	0	1	0
			2959	1899	504	539	17			
1	D	375	Total	C	N	O	S	0	0	0
			2954	1896	504	537	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P14902
A	0	GLY	-	expression tag	UNP P14902
A	1	SER	-	expression tag	UNP P14902
A	2	SER	-	expression tag	UNP P14902
A	3	HIS	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
A	5	HIS	-	expression tag	UNP P14902
A	6	HIS	-	expression tag	UNP P14902
A	7	HIS	-	expression tag	UNP P14902
A	8	HIS	-	expression tag	UNP P14902
A	9	SER	-	expression tag	UNP P14902
A	10	SER	-	expression tag	UNP P14902
A	11	GLY	-	expression tag	UNP P14902
A	12	SER	-	expression tag	UNP P14902
A	13	ALA	-	expression tag	UNP P14902
A	14	ALA	-	expression tag	UNP P14902
A	116	ALA	LYS	engineered mutation	UNP P14902
A	117	ALA	LYS	engineered mutation	UNP P14902
B	-1	MET	-	initiating methionine	UNP P14902
B	0	GLY	-	expression tag	UNP P14902
B	1	SER	-	expression tag	UNP P14902

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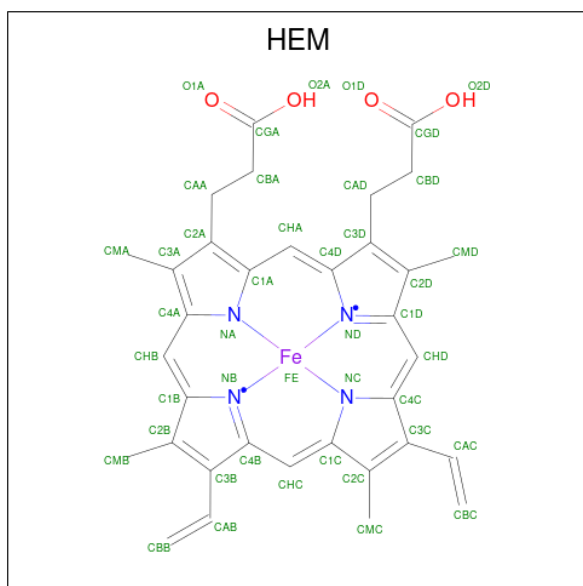
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	9	SER	-	expression tag	UNP P14902
B	10	SER	-	expression tag	UNP P14902
B	11	GLY	-	expression tag	UNP P14902
B	12	SER	-	expression tag	UNP P14902
B	13	ALA	-	expression tag	UNP P14902
B	14	ALA	-	expression tag	UNP P14902
B	116	ALA	LYS	engineered mutation	UNP P14902
B	117	ALA	LYS	engineered mutation	UNP P14902
C	-1	MET	-	initiating methionine	UNP P14902
C	0	GLY	-	expression tag	UNP P14902
C	1	SER	-	expression tag	UNP P14902
C	2	SER	-	expression tag	UNP P14902
C	3	HIS	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
C	5	HIS	-	expression tag	UNP P14902
C	6	HIS	-	expression tag	UNP P14902
C	7	HIS	-	expression tag	UNP P14902
C	8	HIS	-	expression tag	UNP P14902
C	9	SER	-	expression tag	UNP P14902
C	10	SER	-	expression tag	UNP P14902
C	11	GLY	-	expression tag	UNP P14902
C	12	SER	-	expression tag	UNP P14902
C	13	ALA	-	expression tag	UNP P14902
C	14	ALA	-	expression tag	UNP P14902
C	116	ALA	LYS	engineered mutation	UNP P14902
C	117	ALA	LYS	engineered mutation	UNP P14902
D	-1	MET	-	initiating methionine	UNP P14902
D	0	GLY	-	expression tag	UNP P14902
D	1	SER	-	expression tag	UNP P14902
D	2	SER	-	expression tag	UNP P14902
D	3	HIS	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902
D	5	HIS	-	expression tag	UNP P14902
D	6	HIS	-	expression tag	UNP P14902
D	7	HIS	-	expression tag	UNP P14902

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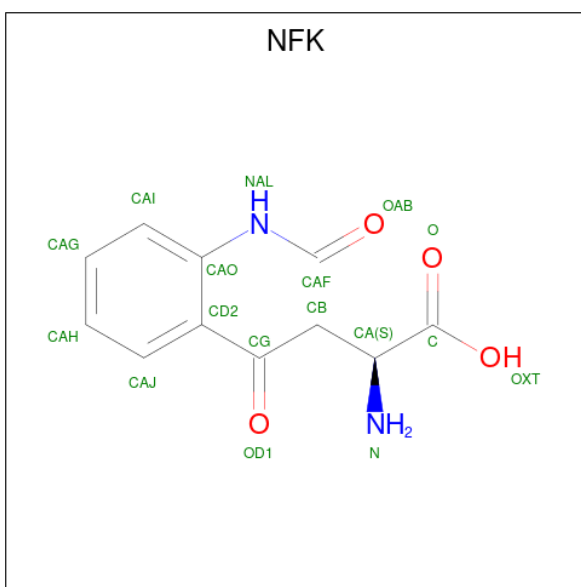
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
D	116	ALA	LYS	engineered mutation	UNP P14902
D	117	ALA	LYS	engineered mutation	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



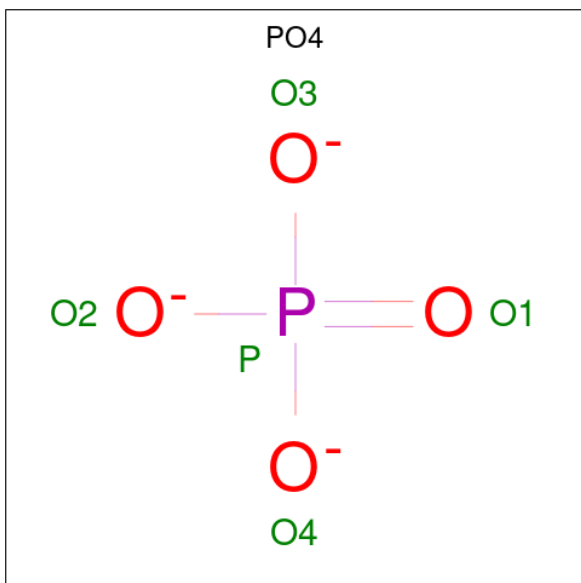
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is N'-Formylkynurenine (CCD ID: NFK) (formula: $C_{11}H_{12}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



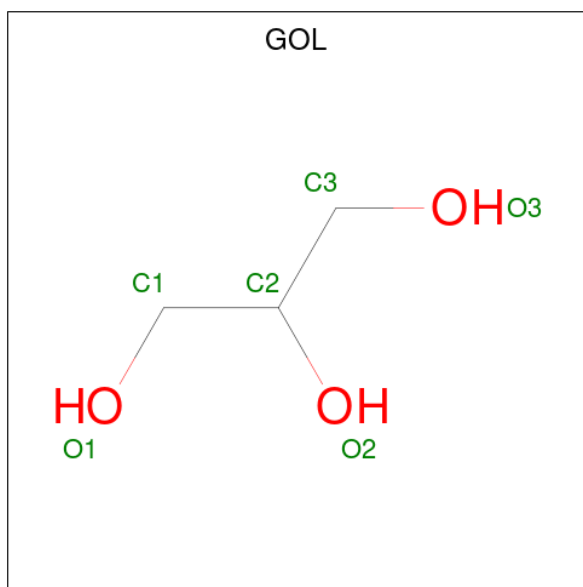
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	11	2	4		
3	C	1	Total	C	N	O	0	0
			17	11	2	4		
3	D	1	Total	C	N	O	0	0
			17	11	2	4		
3	D	1	Total	C	N	O	0	0
			17	11	2	4		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



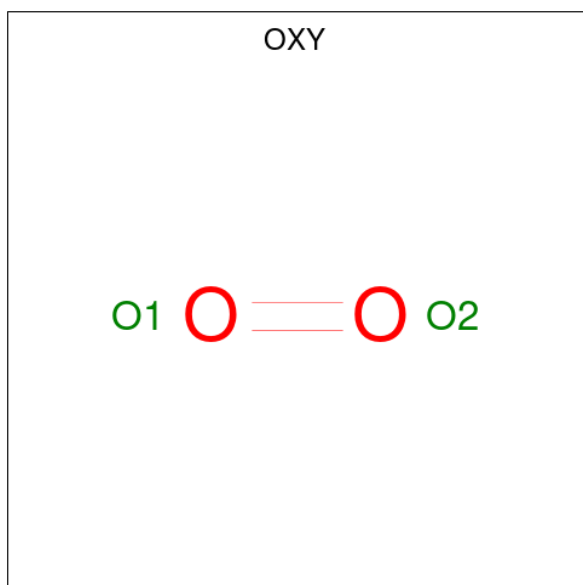
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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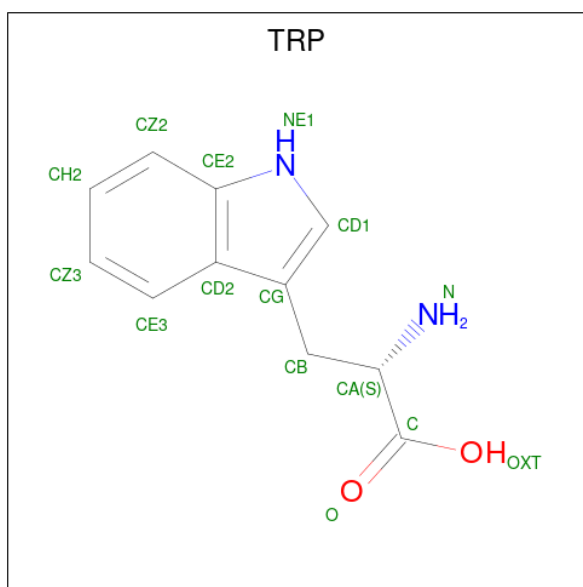
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	D	1	Total O 2 2	0	0

- Molecule 7 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0

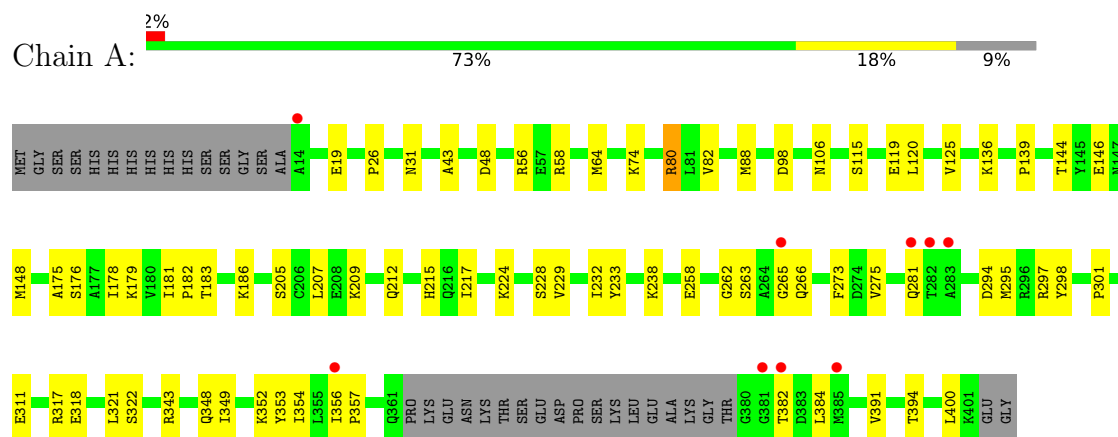
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	118	Total 118	O 118	0	0
9	B	134	Total 134	O 134	0	0
9	C	124	Total 124	O 124	0	0
9	D	116	Total 116	O 116	0	0

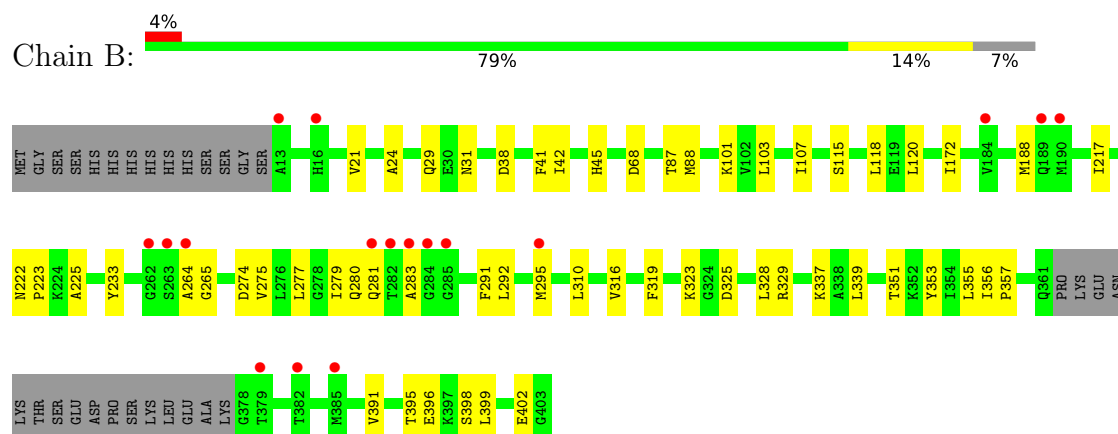
3 Residue-property plots [i](#)

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.

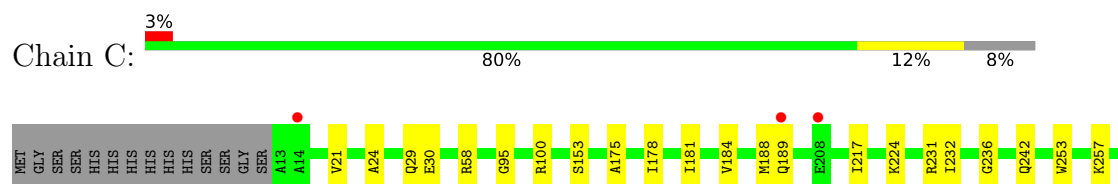
• Molecule 1: Indoleamine 2,3-dioxygenase 1

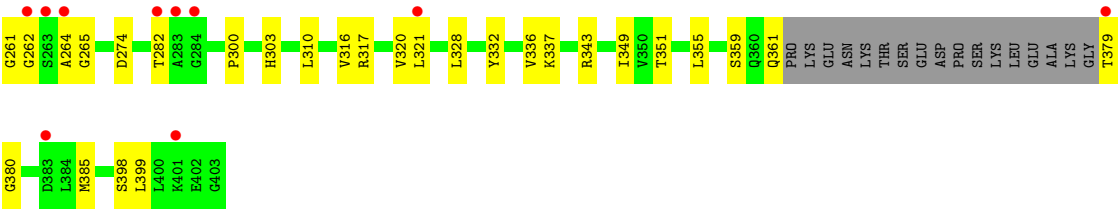


• Molecule 1: Indoleamine 2,3-dioxygenase 1

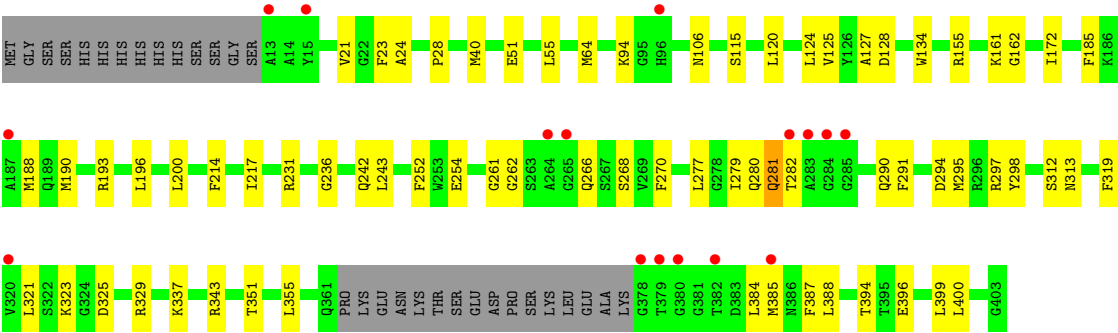
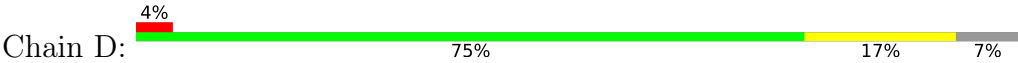


• Molecule 1: Indoleamine 2,3-dioxygenase 1





● Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.36Å 114.57Å 220.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.50 49.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.29-2.50) 99.4 (49.29-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.279 0.216 , 0.276	Depositor DCC
R_{free} test set	3590 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12712	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1345e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, PO4, HEM, CL, NFK, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/2992	0.57	0/4050
1	B	0.38	0/3022	0.56	0/4089
1	C	0.38	0/3027	0.60	0/4096
1	D	0.40	0/3022	0.61	0/4089
All	All	0.38	0/12063	0.58	0/16324

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2924	0	2932	56	0
1	B	2954	0	2956	38	0
1	C	2959	0	2958	39	0
1	D	2954	0	2956	56	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	17	0	0	2	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	34	0	0	1	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	36	0	48	2	0
5	B	36	0	48	1	0
5	C	42	0	56	3	0
5	D	12	0	16	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	C	15	0	9	10	0
7	D	30	0	18	5	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	118	0	0	5	0
9	B	134	0	0	1	0
9	C	124	0	0	4	0
9	D	116	0	0	2	0
All	All	12712	0	12117	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (198) 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:355:LEU:HD11	1:C:385:MET:HE2	1.55	0.87
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.61	0.80
1:D:193:ARG:HG3	1:D:323:LYS:NZ	1.96	0.80
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.63	0.80
1:A:19:GLU:OE2	9:A:601:HOH:O	2.02	0.77
1:A:356:ILE:HG12	1:A:357:PRO:HD3	1.66	0.76
1:D:323:LYS:NZ	1:D:325:ASP:OD2	2.19	0.75
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.71	0.71
1:B:101:LYS:H	5:B:506:GOL:H32	1.55	0.71
1:A:119:GLU:HB2	1:A:301:PRO:HG3	1.73	0.71
1:C:231:ARG:HD2	7:C:503:TRP:O	1.91	0.71
1:D:94:LYS:HB2	5:D:507:GOL:H32	1.72	0.70
1:D:193:ARG:HG3	1:D:323:LYS:HZ2	1.52	0.70
1:D:161:LYS:HB3	7:D:505:TRP:CD1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:HE	1:B:402:GLU:HG3	1.58	0.68
1:C:300:PRO:HG2	1:C:303:HIS:ND1	2.08	0.68
1:C:231:ARG:CD	7:C:503:TRP:O	2.42	0.68
1:D:262:GLY:HA3	1:D:266:GLN:NE2	2.10	0.67
1:A:382:THR:HG22	1:A:384:LEU:H	1.60	0.66
1:C:231:ARG:HD2	7:C:503:TRP:OXT	1.95	0.66
1:C:262:GLY:HA2	7:C:503:TRP:HE1	1.61	0.65
1:C:320:VAL:HG13	1:C:328:LEU:HB3	1.78	0.65
1:C:231:ARG:HD2	7:C:503:TRP:C	2.23	0.64
1:A:175:ALA:HA	1:A:178:ILE:HD12	1.82	0.62
1:B:329:ARG:NE	1:B:402:GLU:HG3	2.13	0.61
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	1.81	0.61
1:D:190:MET:SD	1:D:190:MET:N	2.73	0.61
1:B:274:ASP:OD2	1:B:281:GLN:HG3	2.01	0.61
1:D:161:LYS:HB3	7:D:505:TRP:HD1	1.67	0.60
1:C:175:ALA:HA	1:C:178:ILE:HD12	1.83	0.60
1:D:355:LEU:HD11	1:D:385:MET:HG3	1.84	0.59
1:D:281:GLN:HA	1:D:394:THR:HG21	1.84	0.59
1:C:262:GLY:HA2	7:C:503:TRP:NE1	2.17	0.59
1:B:217:ILE:CD1	2:B:501:HEM:HBB1	2.32	0.59
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.84	0.59
1:A:48:ASP:OD2	9:A:602:HOH:O	2.16	0.59
1:B:41:PHE:O	1:B:45:HIS:HD2	1.86	0.58
1:D:313:ASN:O	9:D:601:HOH:O	2.17	0.58
1:B:115:SER:HB3	1:B:120:LEU:O	2.03	0.58
1:B:265:GLY:HA2	2:B:501:HEM:C4D	2.38	0.58
1:A:262:GLY:HA2	1:A:266:GLN:HE22	1.67	0.57
1:B:337:LYS:HG3	1:B:399:LEU:HD21	1.86	0.57
1:C:100:ARG:HA	5:C:509:GOL:H32	1.86	0.57
1:D:254:GLU:HG3	7:D:504:TRP:O	2.05	0.57
1:D:115:SER:HB3	1:D:120:LEU:O	2.05	0.57
1:D:196:LEU:O	1:D:200:LEU:HG	2.04	0.56
1:D:270:PHE:HB3	1:D:343:ARG:NH2	2.19	0.56
1:A:348:GLN:NE2	3:D:503:NFK:O	2.35	0.56
1:A:281:GLN:NE2	1:A:391:VAL:O	2.39	0.55
1:D:351:THR:HA	1:D:355:LEU:HB2	1.88	0.55
1:A:321:LEU:HD13	1:A:400:LEU:HD13	1.89	0.55
1:D:193:ARG:HG3	1:D:323:LYS:HZ1	1.71	0.55
1:A:263:SER:OG	2:A:501:HEM:O1A	2.22	0.55
1:C:351:THR:HG23	1:C:355:LEU:HD12	1.88	0.55
1:B:277:LEU:HB2	1:B:279:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:THR:HA	1:A:186:LYS:HE2	1.89	0.54
1:B:279:ILE:HG22	1:B:281:GLN:HG2	1.88	0.54
1:A:182:PRO:O	1:A:186:LYS:HG3	2.07	0.54
1:A:56:ARG:H	3:A:502:NFK:CAG	2.21	0.53
1:A:294:ASP:HA	1:A:297:ARG:NH2	2.24	0.53
1:A:64:MET:HE2	1:A:106:ASN:HD22	1.72	0.53
1:A:64:MET:HB2	1:A:106:ASN:ND2	2.24	0.53
1:A:98:ASP:HB3	3:A:502:NFK:C	2.38	0.53
1:A:265:GLY:HA2	2:A:501:HEM:C3D	2.44	0.53
1:D:384:LEU:O	1:D:388:LEU:HD23	2.09	0.53
1:C:58:ARG:NH1	9:C:601:HOH:O	2.12	0.53
1:D:23:PHE:CE2	1:D:268:SER:HB2	2.43	0.53
1:D:94:LYS:HE3	5:D:507:GOL:H12	1.91	0.53
1:D:387:PHE:HD2	1:D:388:LEU:HD22	1.74	0.53
1:A:31:ASN:ND2	5:A:507:GOL:O3	2.40	0.53
1:D:355:LEU:HD11	1:D:385:MET:CG	2.40	0.52
1:A:238:LYS:HA	1:A:258:GLU:HB3	1.90	0.52
1:A:176:SER:HA	1:A:179:LYS:HE2	1.91	0.52
1:C:153:SER:HB2	5:C:505:GOL:H32	1.91	0.52
1:D:294:ASP:OD1	1:D:297:ARG:HD3	2.10	0.52
1:A:266:GLN:HG2	1:A:298:TYR:HB2	1.91	0.51
1:B:87:THR:HG23	1:B:103:LEU:HD13	1.93	0.51
1:D:124:LEU:HD12	1:D:128:ASP:HB2	1.92	0.50
1:D:217:ILE:CD1	2:D:501:HEM:HBB1	2.41	0.50
1:A:88:MET:HG3	1:A:233:TYR:O	2.12	0.50
1:D:387:PHE:CD2	1:D:388:LEU:HD22	2.46	0.50
1:B:319:PHE:O	1:B:323:LYS:HG2	2.12	0.50
1:C:21:VAL:HB	1:C:24:ALA:HB3	1.94	0.50
1:D:313:ASN:N	1:D:313:ASN:HD22	2.09	0.49
1:D:321:LEU:HD13	1:D:400:LEU:HD22	1.94	0.49
1:A:352:LYS:HD3	1:A:353:TYR:CE2	2.47	0.49
1:A:178:ILE:HA	1:A:181:ILE:HG13	1.95	0.49
1:D:94:LYS:HG3	5:D:507:GOL:H12	1.95	0.48
1:C:58:ARG:HD2	9:C:601:HOH:O	2.13	0.48
1:B:351:THR:HA	1:B:355:LEU:HB2	1.96	0.48
1:C:29:GLN:O	1:C:30:GLU:HB2	2.13	0.48
1:D:51:GLU:OE2	1:D:155:ARG:NH2	2.35	0.48
1:D:236:GLY:HA3	1:D:261:GLY:N	2.29	0.47
1:C:178:ILE:HA	1:C:181:ILE:HG13	1.96	0.47
1:D:55:LEU:O	1:D:55:LEU:HG	2.08	0.47
1:A:281:GLN:NE2	1:A:394:THR:HB	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLN:HG3	1:B:283:ALA:HB3	1.96	0.47
1:C:264:ALA:H	7:C:503:TRP:HZ2	1.63	0.47
1:C:316:VAL:O	1:C:320:VAL:HG23	2.15	0.47
1:A:262:GLY:HA2	1:A:266:GLN:NE2	2.29	0.47
1:A:58:ARG:NH1	9:A:605:HOH:O	2.43	0.46
1:A:354:ILE:C	1:A:357:PRO:HD2	2.40	0.46
1:D:21:VAL:HB	1:D:24:ALA:HB3	1.97	0.46
1:A:19:GLU:H	1:A:19:GLU:CD	2.23	0.46
5:C:505:GOL:O1	5:C:505:GOL:O3	2.33	0.46
1:D:125:VAL:HG23	1:D:127:ALA:H	1.80	0.46
1:A:106:ASN:HB2	9:A:644:HOH:O	2.15	0.46
1:A:80:ARG:HH21	1:A:125:VAL:HG22	1.80	0.46
1:A:136:LYS:HD3	1:A:139:PRO:HA	1.97	0.46
1:C:274:ASP:CG	1:C:343:ARG:HH22	2.24	0.46
1:D:294:ASP:O	1:D:297:ARG:HB2	2.15	0.46
1:D:21:VAL:HG12	1:D:172:ILE:HG12	1.97	0.46
1:A:144:THR:O	1:A:148:MET:HG3	2.17	0.45
1:B:325:ASP:HB3	1:B:328:LEU:HB2	1.99	0.45
1:B:281:GLN:NE2	1:B:391:VAL:HG13	2.32	0.45
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.98	0.45
1:B:21:VAL:HB	1:B:24:ALA:HB3	1.98	0.45
1:C:343:ARG:HD3	2:C:501:HEM:O2D	2.17	0.45
1:C:359:SER:C	1:C:361:GLN:H	2.24	0.45
1:C:217:ILE:HG21	1:C:349:ILE:HD12	1.98	0.45
1:B:29:GLN:NE2	1:B:31:ASN:O	2.43	0.45
1:B:188:MET:HE3	1:B:319:PHE:HB2	1.97	0.45
1:C:379:THR:HG22	1:C:380:GLY:H	1.82	0.45
1:D:266:GLN:HG2	1:D:298:TYR:HB2	1.99	0.45
1:A:275:VAL:HG13	1:A:311:GLU:HG3	1.98	0.44
1:D:185:PHE:HD1	1:D:188:MET:HE1	1.81	0.44
1:A:217:ILE:HD11	2:A:501:HEM:HBB1	1.99	0.44
1:A:263:SER:HB3	1:A:265:GLY:H	1.83	0.44
1:A:212:GLN:O	1:A:215:HIS:HB2	2.18	0.44
1:B:265:GLY:O	9:B:601:HOH:O	2.21	0.44
1:D:277:LEU:HB2	1:D:279:ILE:CD1	2.48	0.44
1:B:264:ALA:HB1	2:B:501:HEM:C1C	2.53	0.44
1:B:88:MET:HG3	1:B:233:TYR:O	2.18	0.44
1:C:332:TYR:O	1:C:336:VAL:HG23	2.17	0.44
1:A:317:ARG:O	1:A:321:LEU:HB2	2.18	0.44
1:B:188:MET:SD	1:B:316:VAL:HG22	2.58	0.43
1:D:280:GLN:O	1:D:282:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:GLU:O	1:D:399:LEU:HD12	2.18	0.43
1:B:223:PRO:HA	1:B:353:TYR:CD1	2.53	0.43
1:B:107:ILE:HD12	1:B:107:ILE:HG23	1.82	0.43
1:A:275:VAL:CG1	1:A:311:GLU:HG3	2.49	0.43
1:C:189:GLN:NE2	9:C:603:HOH:O	2.37	0.43
1:D:64:MET:HB2	1:D:106:ASN:ND2	2.34	0.43
1:B:217:ILE:HD13	2:B:501:HEM:HBB1	2.00	0.43
7:C:503:TRP:HB2	9:C:672:HOH:O	2.19	0.43
1:D:262:GLY:HA3	1:D:266:GLN:CD	2.44	0.43
1:D:231:ARG:HD2	9:D:693:HOH:O	2.18	0.43
1:D:325:ASP:O	1:D:329:ARG:HG3	2.19	0.43
1:A:266:GLN:HG3	1:A:295:MET:HE3	2.00	0.42
1:B:275:VAL:HG11	1:B:310:LEU:HB3	2.01	0.42
1:D:40:MET:HE2	1:D:40:MET:HB2	1.68	0.42
1:B:291:PHE:CZ	2:B:501:HEM:HBA1	2.54	0.42
1:A:294:ASP:OD1	1:A:297:ARG:NH2	2.52	0.42
1:D:214:PHE:O	1:D:214:PHE:HD1	2.02	0.42
1:A:115:SER:HB3	1:A:120:LEU:O	2.19	0.42
1:B:21:VAL:HG12	1:B:172:ILE:HG12	2.01	0.42
1:C:265:GLY:HA2	2:C:501:HEM:C3D	2.53	0.42
1:C:184:VAL:O	1:C:188:MET:HG3	2.19	0.42
1:C:231:ARG:O	1:C:231:ARG:HG2	2.17	0.42
1:A:229:VAL:O	1:A:232:ILE:HG12	2.19	0.42
1:D:188:MET:HE2	1:D:188:MET:HB3	1.59	0.42
1:A:43:ALA:HB2	1:A:82:VAL:HG13	2.00	0.42
1:A:224:LYS:HE2	1:A:228:SER:OG	2.19	0.42
1:A:322:SER:HB3	9:A:674:HOH:O	2.19	0.42
1:B:356:ILE:HB	1:B:357:PRO:HD3	2.01	0.42
7:C:503:TRP:HA	7:C:503:TRP:CE3	2.54	0.42
1:B:396:GLU:C	1:B:398:SER:H	2.28	0.42
1:D:185:PHE:HA	1:D:188:MET:HE2	2.02	0.41
1:C:95:GLY:HA3	1:C:232:ILE:HD13	2.02	0.41
1:C:236:GLY:HA3	1:C:261:GLY:N	2.35	0.41
1:D:242:GLN:O	1:D:243:LEU:HD23	2.21	0.41
1:B:339:LEU:HG	1:B:395:THR:HG21	2.03	0.41
1:D:291:PHE:CE2	1:D:295:MET:HE3	2.55	0.41
1:D:337:LYS:HG3	1:D:399:LEU:HD21	2.01	0.41
1:A:26:PRO:O	1:A:74:LYS:NZ	2.48	0.41
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.86	0.41
1:C:337:LYS:HG3	1:C:399:LEU:HD21	2.03	0.41
1:D:162:GLY:H	7:D:505:TRP:CD1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:TRP:CG	1:C:257:LYS:HE2	2.56	0.41
1:D:28:PRO:HD3	1:D:134:TRP:CZ2	2.56	0.41
1:A:146:GLU:H	1:A:146:GLU:CD	2.29	0.41
1:B:222:ASN:OD1	1:B:225:ALA:N	2.44	0.41
1:B:291:PHE:CE2	1:B:295:MET:HE3	2.56	0.41
1:C:317:ARG:NH1	1:C:398:SER:O	2.33	0.41
1:D:188:MET:HG2	1:D:319:PHE:CD2	2.56	0.41
1:C:321:LEU:HA	1:C:321:LEU:HD23	1.82	0.41
1:A:31:ASN:OD1	5:A:507:GOL:H11	2.20	0.40
1:A:207:LEU:HD21	1:A:273:PHE:CE2	2.55	0.40
1:A:321:LEU:HD12	1:A:321:LEU:HA	1.62	0.40
1:A:343:ARG:HD3	2:A:501:HEM:O2D	2.21	0.40
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.80	0.40
1:D:252:PHE:O	7:D:504:TRP:HB2	2.22	0.40
1:C:262:GLY:CA	7:C:503:TRP:HE1	2.33	0.40
1:A:205:SER:O	1:A:209:LYS:HG3	2.22	0.40
1:A:217:ILE:HG21	1:A:349:ILE:HD12	2.03	0.40
1:B:292:LEU:HD23	1:B:292:LEU:HA	2.00	0.40
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.91	0.40
1:B:38:ASP:O	1:B:42:ILE:HG13	2.22	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	366/405 (90%)	345 (94%)	21 (6%)	0	100	100
1	B	371/405 (92%)	354 (95%)	17 (5%)	0	100	100
1	C	371/405 (92%)	350 (94%)	21 (6%)	0	100	100
1	D	371/405 (92%)	342 (92%)	27 (7%)	2 (0%)	24	43
All	All	1479/1620 (91%)	1391 (94%)	86 (6%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	GLN
1	D	312	SER

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	317/346 (92%)	315 (99%)	2 (1%)	78	91
1	B	319/346 (92%)	318 (100%)	1 (0%)	86	94
1	C	320/346 (92%)	317 (99%)	3 (1%)	70	87
1	D	319/346 (92%)	318 (100%)	1 (0%)	86	94
All	All	1275/1384 (92%)	1268 (100%)	7 (0%)	76	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	318	GLU
1	B	68	ASP
1	C	224	LYS
1	C	242	GLN
1	C	282	THR
1	D	290	GLN

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

Mol	Chain	Res	Type
1	A	106	ASN
1	B	45	HIS
1	B	73	HIS
1	C	31	ASN
1	C	106	ASN
1	C	191	GLN

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Mol	Chain	Res	Type
1	D	29	GLN
1	D	106	ASN
1	D	220	HIS
1	D	290	GLN
1	D	313	ASN
1	D	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	C	507	-	5,5,5	0.58	0	5,5,5	0.19	0
7	TRP	D	505	-	15,16,16	2.07	4 (26%)	18,22,22	1.45	3 (16%)
2	HEM	D	501	1	50,50,50	1.66	7 (14%)	67,82,82	1.66	12 (17%)
4	PO4	A	503	-	4,4,4	0.94	0	6,6,6	1.06	0
3	NFK	D	503	-	16,17,17	2.49	3 (18%)	16,22,22	1.68	2 (12%)
5	GOL	A	505	-	5,5,5	0.41	0	5,5,5	0.76	0
5	GOL	A	506	-	5,5,5	0.47	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	505	-	5,5,5	0.47	0	5,5,5	0.32	0
2	HEM	B	501	1	50,50,50	1.61	5 (10%)	67,82,82	1.44	7 (10%)
6	OXY	B	508	-	1,1,1	0.33	0	-		
6	OXY	D	509	-	1,1,1	0.34	0	-		
5	GOL	D	506	-	5,5,5	0.48	0	5,5,5	0.79	0
7	TRP	C	503	-	15,16,16	1.90	3 (20%)	18,22,22	1.28	3 (16%)
5	GOL	C	509	-	5,5,5	0.55	0	5,5,5	0.38	0
2	HEM	A	501	1	50,50,50	1.62	9 (18%)	67,82,82	1.63	14 (20%)
5	GOL	A	509	-	5,5,5	0.56	0	5,5,5	0.51	0
7	TRP	D	504	-	15,16,16	1.92	4 (26%)	18,22,22	1.34	2 (11%)
4	PO4	C	504	-	4,4,4	0.75	0	6,6,6	0.84	0
5	GOL	C	510	-	5,5,5	0.54	0	5,5,5	0.38	0
3	NFK	A	502	-	16,17,17	2.75	4 (25%)	16,22,22	2.24	6 (37%)
3	NFK	D	502	-	16,17,17	2.63	5 (31%)	16,22,22	3.15	6 (37%)
2	HEM	C	501	1	50,50,50	1.59	9 (18%)	67,82,82	1.55	10 (14%)
5	GOL	B	502	-	5,5,5	0.53	0	5,5,5	0.39	0
5	GOL	B	504	-	5,5,5	0.50	0	5,5,5	0.50	0
3	NFK	C	502	-	16,17,17	2.78	4 (25%)	16,22,22	1.66	3 (18%)
5	GOL	B	503	-	5,5,5	0.46	0	5,5,5	0.71	0
5	GOL	A	508	-	5,5,5	0.53	0	5,5,5	0.26	0
5	GOL	B	507	-	5,5,5	0.57	0	5,5,5	0.41	0
5	GOL	C	508	-	5,5,5	0.59	0	5,5,5	0.67	0
5	GOL	C	506	-	5,5,5	0.54	0	5,5,5	0.26	0
5	GOL	B	505	-	5,5,5	0.49	0	5,5,5	0.36	0
5	GOL	A	504	-	5,5,5	0.52	0	5,5,5	0.37	0
5	GOL	D	507	-	5,5,5	0.51	0	5,5,5	0.36	0
5	GOL	C	511	-	5,5,5	0.39	0	5,5,5	1.10	0
6	OXY	A	510	-	1,1,1	0.34	0	-		
5	GOL	B	506	-	5,5,5	0.50	0	5,5,5	0.78	0
5	GOL	A	507	-	5,5,5	0.41	0	5,5,5	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	507	-	-	3/4/4/4	-
7	TRP	D	505	-	-	6/8/8/8	0/2/2/2
2	HEM	D	501	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NFK	D	503	-	-	8/15/15/15	0/1/1/1
5	GOL	A	505	-	-	0/4/4/4	-
5	GOL	A	506	-	-	0/4/4/4	-
5	GOL	C	505	-	-	2/4/4/4	-
2	HEM	B	501	1	-	3/14/54/54	-
5	GOL	D	506	-	-	2/4/4/4	-
7	TRP	C	503	-	-	6/8/8/8	0/2/2/2
5	GOL	C	509	-	-	0/4/4/4	-
2	HEM	A	501	1	-	6/14/54/54	-
5	GOL	A	509	-	-	2/4/4/4	-
7	TRP	D	504	-	-	4/8/8/8	0/2/2/2
5	GOL	C	510	-	-	0/4/4/4	-
3	NFK	A	502	-	-	6/15/15/15	0/1/1/1
3	NFK	D	502	-	-	7/15/15/15	0/1/1/1
2	HEM	C	501	1	-	6/14/54/54	-
5	GOL	B	502	-	-	2/4/4/4	-
5	GOL	B	504	-	-	0/4/4/4	-
3	NFK	C	502	-	-	8/15/15/15	0/1/1/1
5	GOL	B	503	-	-	2/4/4/4	-
5	GOL	A	508	-	-	2/4/4/4	-
5	GOL	B	507	-	-	3/4/4/4	-
5	GOL	C	508	-	-	0/4/4/4	-
5	GOL	C	506	-	-	0/4/4/4	-
5	GOL	B	505	-	-	1/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-
5	GOL	D	507	-	-	3/4/4/4	-
5	GOL	C	511	-	-	0/4/4/4	-
5	GOL	B	506	-	-	2/4/4/4	-
5	GOL	A	507	-	-	1/4/4/4	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NFK	CAF-NAL	9.50	1.46	1.34
3	C	502	NFK	CAF-NAL	9.46	1.46	1.34
3	D	502	NFK	CAF-NAL	8.61	1.45	1.34
3	D	503	NFK	CAF-NAL	8.32	1.45	1.34
2	B	501	HEM	FE-ND	7.00	2.16	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-ND	6.23	2.14	1.94
7	D	505	TRP	CB-CG	5.97	1.61	1.50
2	A	501	HEM	FE-NC	5.79	2.14	1.95
7	D	504	TRP	CB-CG	5.46	1.60	1.50
7	C	503	TRP	CB-CG	5.27	1.60	1.50
2	C	501	HEM	FE-ND	4.79	2.09	1.94
2	D	501	HEM	FE-NC	4.73	2.10	1.95
2	A	501	HEM	FE-NB	4.56	2.09	1.94
2	C	501	HEM	FE-NA	4.38	2.09	1.95
3	D	502	NFK	CD2-CG	3.96	1.56	1.48
3	C	502	NFK	CAO-NAL	3.82	1.47	1.41
2	B	501	HEM	FE-NA	3.67	2.07	1.95
2	C	501	HEM	FE-NC	3.63	2.07	1.95
3	A	502	NFK	CAO-NAL	3.56	1.46	1.41
3	D	503	NFK	CAO-NAL	3.30	1.46	1.41
2	D	501	HEM	FE-NA	3.25	2.05	1.95
2	D	501	HEM	CAB-C3B	3.19	1.55	1.47
2	A	501	HEM	FE-ND	3.16	2.04	1.94
2	D	501	HEM	CAC-C3C	3.14	1.55	1.47
2	B	501	HEM	CAC-C3C	3.11	1.55	1.47
2	A	501	HEM	CAC-C3C	3.02	1.55	1.47
2	C	501	HEM	CAC-C3C	3.00	1.55	1.47
2	B	501	HEM	CAB-C3B	2.96	1.55	1.47
2	C	501	HEM	CAB-C3B	2.85	1.55	1.47
7	D	505	TRP	O-C	2.79	1.30	1.22
3	C	502	NFK	OD1-CG	-2.66	1.17	1.22
3	D	503	NFK	CD2-CG	2.64	1.53	1.48
3	D	502	NFK	CAO-NAL	2.54	1.45	1.41
3	A	502	NFK	OD1-CG	-2.52	1.18	1.22
2	A	501	HEM	FE-NA	2.50	2.03	1.95
2	A	501	HEM	CMC-C2C	2.42	1.55	1.50
7	C	503	TRP	CD1-NE1	-2.42	1.33	1.37
7	D	505	TRP	CD1-NE1	-2.41	1.33	1.37
7	D	505	TRP	CD1-CG	2.40	1.40	1.36
2	A	501	HEM	CAB-C3B	2.38	1.53	1.47
2	D	501	HEM	FE-NB	2.38	2.02	1.94
2	A	501	HEM	C3B-C2B	-2.37	1.32	1.37
2	C	501	HEM	CMA-C3A	2.35	1.55	1.50
2	B	501	HEM	CMC-C2C	2.28	1.55	1.50
3	A	502	NFK	CD2-CG	2.26	1.53	1.48
7	D	504	TRP	O-C	2.23	1.28	1.22
2	C	501	HEM	FE-NB	2.19	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NFK	CB-CG	2.17	1.54	1.51
7	D	504	TRP	CD1-CG	2.16	1.40	1.36
2	D	501	HEM	CMC-C2C	2.09	1.55	1.50
7	C	503	TRP	CD2-CE2	-2.07	1.38	1.41
2	C	501	HEM	CMD-C2D	2.07	1.55	1.50
3	C	502	NFK	CD2-CG	2.04	1.52	1.48
2	A	501	HEM	CMA-C3A	2.03	1.54	1.50
3	D	502	NFK	OD1-CG	-2.03	1.18	1.22
2	C	501	HEM	CMC-C2C	2.02	1.54	1.50
7	D	504	TRP	CD2-CE2	-2.00	1.38	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NFK	CA-CB-CG	9.63	123.34	113.06
3	A	502	NFK	CB-CG-CD2	5.67	126.42	119.82
3	D	503	NFK	OAB-CAF-NAL	-5.00	118.85	125.72
2	A	501	HEM	C3B-C4B-NB	-4.61	106.15	109.47
2	D	501	HEM	C3B-C4B-NB	-4.45	106.27	109.47
2	C	501	HEM	C3B-C4B-NB	-4.44	106.28	109.47
2	B	501	HEM	C3B-C4B-NB	-4.22	106.44	109.47
3	D	502	NFK	CAO-NAL-CAF	-4.16	118.53	126.87
2	D	501	HEM	C3B-C2B-C1B	4.14	109.52	106.41
3	D	502	NFK	OAB-CAF-NAL	-3.96	120.28	125.72
2	C	501	HEM	C1B-NB-C4B	3.81	109.72	105.21
2	D	501	HEM	C1B-NB-C4B	3.79	109.70	105.21
2	C	501	HEM	C3B-C2B-C1B	3.75	109.22	106.41
7	D	504	TRP	CA-CB-CG	3.71	120.53	113.49
2	B	501	HEM	C1B-NB-C4B	3.56	109.43	105.21
3	C	502	NFK	CA-CB-CG	-3.52	109.30	113.06
2	A	501	HEM	CAA-CBA-CGA	-3.52	104.34	113.67
3	A	502	NFK	OD1-CG-CD2	-3.44	115.15	120.79
3	D	503	NFK	CAO-NAL-CAF	-3.26	120.34	126.87
2	B	501	HEM	CHD-C4C-NC	3.22	127.96	124.45
2	A	501	HEM	C4D-ND-C1D	3.21	109.01	105.21
7	D	505	TRP	OXT-C-O	-3.14	116.96	124.08
2	D	501	HEM	C2B-C1B-NB	-3.12	106.25	109.84
3	D	502	NFK	CAI-CAO-NAL	-3.03	117.94	122.54
2	D	501	HEM	CHB-C1B-NB	3.00	128.08	124.37
3	C	502	NFK	CB-CG-CD2	3.00	123.31	119.82
3	D	502	NFK	OXT-C-O	-2.99	117.29	124.08
2	A	501	HEM	C2D-C1D-ND	-2.96	106.48	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1B-NB-C4B	2.95	108.70	105.21
2	C	501	HEM	C2B-C1B-NB	-2.91	106.49	109.84
7	D	504	TRP	OXT-C-O	-2.90	117.51	124.08
2	D	501	HEM	CHD-C4C-NC	2.89	127.60	124.45
2	C	501	HEM	CHB-C1B-NB	2.89	127.94	124.37
7	C	503	TRP	OXT-C-O	-2.87	117.56	124.08
2	B	501	HEM	C3B-C2B-C1B	2.78	108.50	106.41
2	D	501	HEM	C2A-C1A-NA	-2.77	107.08	110.15
2	A	501	HEM	CAD-CBD-CGD	-2.72	106.46	113.67
7	D	505	TRP	CD2-CE2-NE1	2.69	109.76	107.52
3	D	502	NFK	CB-CA-N	-2.67	100.72	112.42
2	D	501	HEM	CAA-CBA-CGA	-2.61	106.75	113.67
3	A	502	NFK	CAJ-CD2-CG	-2.57	113.39	119.61
2	B	501	HEM	CHB-C1B-NB	2.57	127.54	124.37
7	D	505	TRP	CD2-CG-CD1	-2.46	103.64	106.16
2	B	501	HEM	C2B-C1B-NB	-2.45	107.02	109.84
2	C	501	HEM	CHD-C4C-NC	2.42	127.09	124.45
2	C	501	HEM	C4D-ND-C1D	2.42	108.08	105.21
2	D	501	HEM	C4D-ND-C1D	2.35	107.99	105.21
2	A	501	HEM	C3D-C4D-ND	-2.35	107.60	110.17
2	A	501	HEM	C3B-C2B-C1B	2.32	108.15	106.41
2	C	501	HEM	CHC-C4B-C3B	2.28	129.62	125.07
3	A	502	NFK	CAI-CAO-NAL	-2.28	119.09	122.54
3	A	502	NFK	CA-CB-CG	-2.28	110.63	113.06
7	C	503	TRP	CA-CB-CG	2.23	117.73	113.49
2	A	501	HEM	C2A-C1A-NA	-2.20	107.71	110.15
2	A	501	HEM	CHB-C1B-NB	2.19	127.08	124.37
2	D	501	HEM	O2D-CGD-CBD	2.18	120.88	114.00
2	A	501	HEM	CHD-C4C-C3C	2.18	128.88	125.21
2	C	501	HEM	C3D-C4D-ND	-2.14	107.82	110.17
3	C	502	NFK	OXT-C-O	-2.13	119.24	124.08
2	D	501	HEM	CAB-C3B-C2B	-2.13	121.52	128.43
2	A	501	HEM	CHC-C1C-NC	2.12	126.76	124.45
7	C	503	TRP	CB-CG-CD2	2.09	130.71	126.70
3	A	502	NFK	CAJ-CD2-CAO	2.08	121.15	118.81
2	B	501	HEM	CAA-CBA-CGA	-2.05	108.22	113.67
2	A	501	HEM	C4B-C3B-C2B	2.04	109.15	107.28
2	D	501	HEM	CHC-C4B-C3B	2.02	129.10	125.07
2	A	501	HEM	C4C-NC-C1C	2.01	109.10	105.82
2	C	501	HEM	C2D-C1D-ND	-2.00	107.59	109.90

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NFK	CAO-CD2-CG-CB
3	A	502	NFK	CAO-CD2-CG-OD1
3	C	502	NFK	O-C-CA-N
3	D	502	NFK	CD2-CAO-NAL-CAF
3	D	502	NFK	CAI-CAO-NAL-CAF
3	D	503	NFK	O-C-CA-N
5	B	506	GOL	O1-C1-C2-C3
5	C	505	GOL	C1-C2-C3-O3
5	D	507	GOL	C1-C2-C3-O3
7	C	503	TRP	O-C-CA-N
7	C	503	TRP	N-CA-CB-CG
7	C	503	TRP	CA-CB-CG-CD2
7	D	505	TRP	N-CA-CB-CG
7	D	505	TRP	CA-CB-CG-CD2
7	C	503	TRP	CA-CB-CG-CD1
7	D	504	TRP	OXT-C-CA-N
7	D	505	TRP	CA-CB-CG-CD1
3	C	502	NFK	CAI-CAO-NAL-CAF
3	D	503	NFK	CAI-CAO-NAL-CAF
5	A	508	GOL	O2-C2-C3-O3
5	C	505	GOL	O2-C2-C3-O3
3	D	503	NFK	OXT-C-CA-N
7	C	503	TRP	OXT-C-CA-N
2	C	501	HEM	C2A-CAA-CBA-CGA
3	C	502	NFK	OXT-C-CA-N
5	A	508	GOL	C1-C2-C3-O3
5	A	509	GOL	C1-C2-C3-O3
5	B	502	GOL	C1-C2-C3-O3
5	B	503	GOL	C1-C2-C3-O3
5	B	507	GOL	C1-C2-C3-O3
5	C	507	GOL	C1-C2-C3-O3
5	D	506	GOL	C1-C2-C3-O3
5	A	509	GOL	O2-C2-C3-O3
5	B	502	GOL	O2-C2-C3-O3
5	B	506	GOL	O1-C1-C2-O2
5	D	506	GOL	O2-C2-C3-O3
5	D	507	GOL	O2-C2-C3-O3
3	D	502	NFK	CA-CB-CG-CD2
3	D	502	NFK	CAJ-CD2-CG-OD1
3	D	502	NFK	CAO-CD2-CG-OD1
2	D	501	HEM	C2A-CAA-CBA-CGA
3	D	502	NFK	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
7	D	505	TRP	C-CA-CB-CG
3	D	503	NFK	CAJ-CD2-CG-OD1
7	D	504	TRP	CA-CB-CG-CD2
3	D	503	NFK	CAJ-CD2-CG-CB
7	D	504	TRP	O-C-CA-N
3	C	502	NFK	CAJ-CD2-CG-OD1
5	B	505	GOL	O1-C1-C2-C3
3	C	502	NFK	CD2-CAO-NAL-CAF
3	D	503	NFK	CD2-CAO-NAL-CAF
2	A	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
7	D	505	TRP	O-C-CA-CB
3	D	503	NFK	CAO-CD2-CG-OD1
5	C	507	GOL	O2-C2-C3-O3
3	C	502	NFK	OXT-C-CA-CB
7	D	505	TRP	OXT-C-CA-CB
2	A	501	HEM	C2A-CAA-CBA-CGA
7	C	503	TRP	C-CA-CB-CG
5	B	503	GOL	O2-C2-C3-O3
5	D	507	GOL	O1-C1-C2-C3
3	C	502	NFK	O-C-CA-CB
7	D	504	TRP	CA-CB-CG-CD1
3	D	503	NFK	CAO-CD2-CG-CB
2	C	501	HEM	C3A-C2A-CAA-CBA
3	D	502	NFK	CAJ-CD2-CG-CB
2	C	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	CAA-CBA-CGA-O1A
5	B	507	GOL	O1-C1-C2-C3
3	A	502	NFK	O-C-CA-N
5	B	507	GOL	O2-C2-C3-O3
2	B	501	HEM	CAA-CBA-CGA-O1A
3	A	502	NFK	OXT-C-CA-N
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
5	A	507	GOL	O1-C1-C2-O2
2	C	501	HEM	CAA-CBA-CGA-O1A
5	C	507	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	502	NFK	O-C-CA-CB
3	C	502	NFK	CAO-CD2-CG-OD1
2	D	501	HEM	CAA-CBA-CGA-O1A
3	A	502	NFK	OXT-C-CA-CB
2	D	501	HEM	CAA-CBA-CGA-O2A

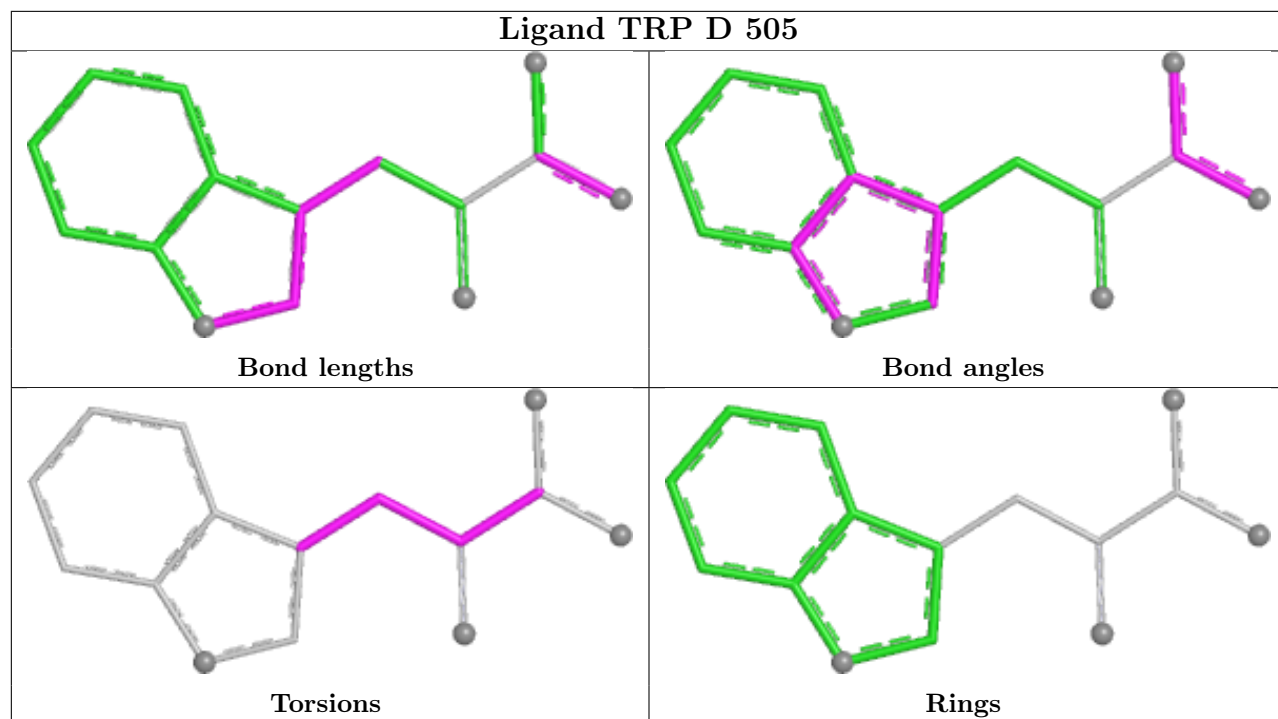
There are no ring outliers.

14 monomers are involved in 45 short contacts:

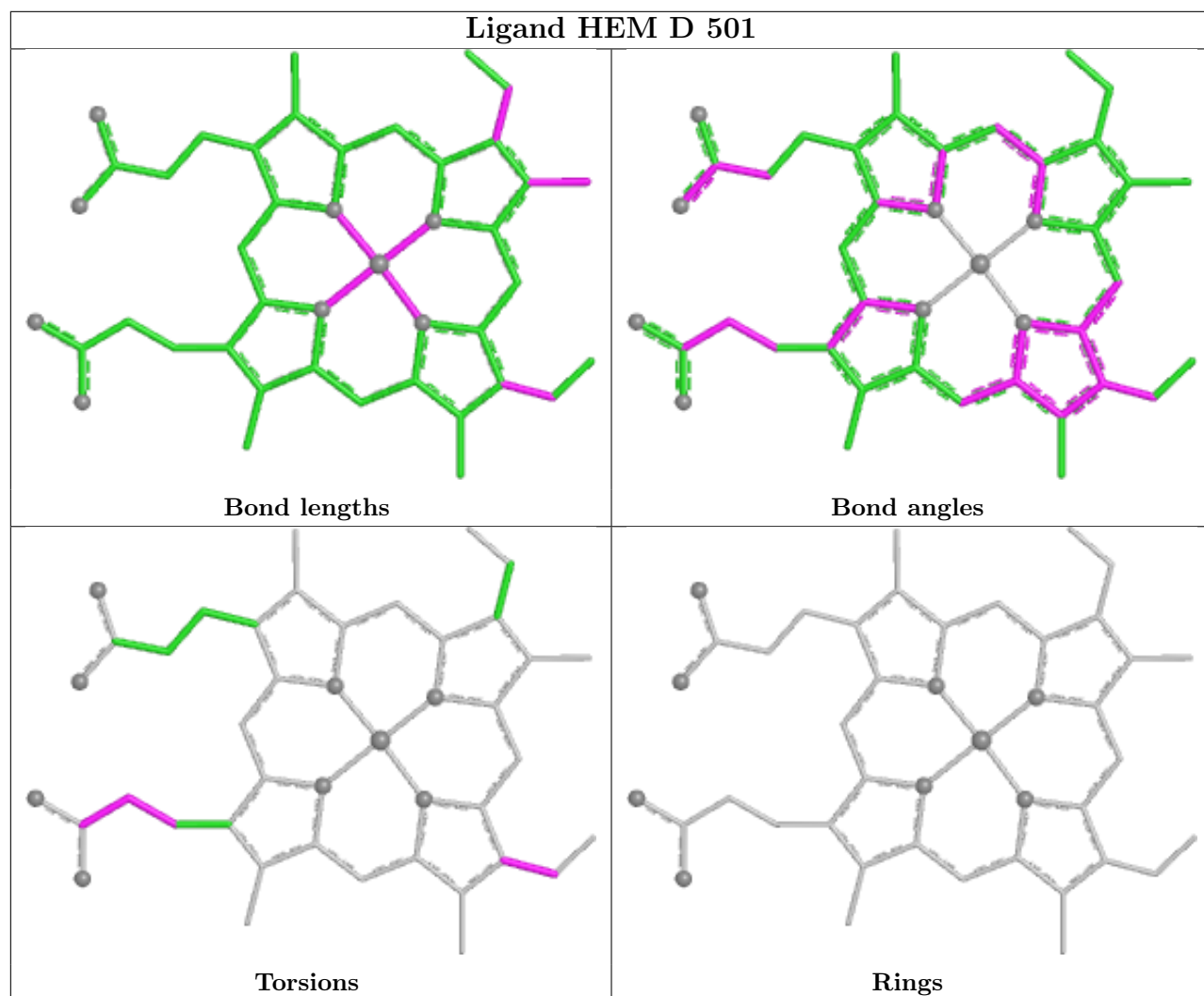
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	505	TRP	3	0
2	D	501	HEM	3	0
3	D	503	NFK	1	0
5	C	505	GOL	2	0
2	B	501	HEM	6	0
7	C	503	TRP	10	0
5	C	509	GOL	1	0
2	A	501	HEM	6	0
7	D	504	TRP	2	0
3	A	502	NFK	2	0
2	C	501	HEM	3	0
5	D	507	GOL	3	0
5	B	506	GOL	1	0
5	A	507	GOL	2	0

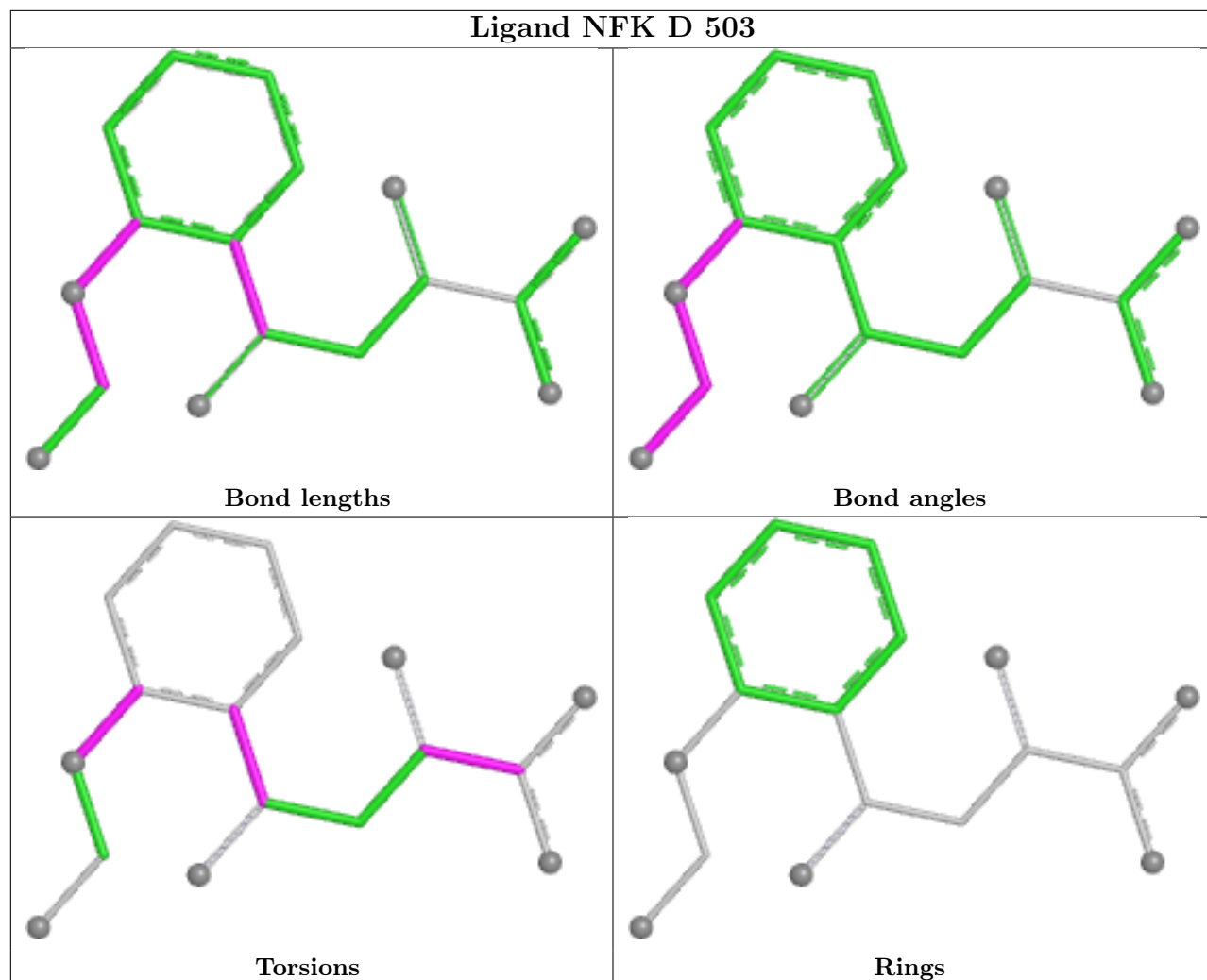
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

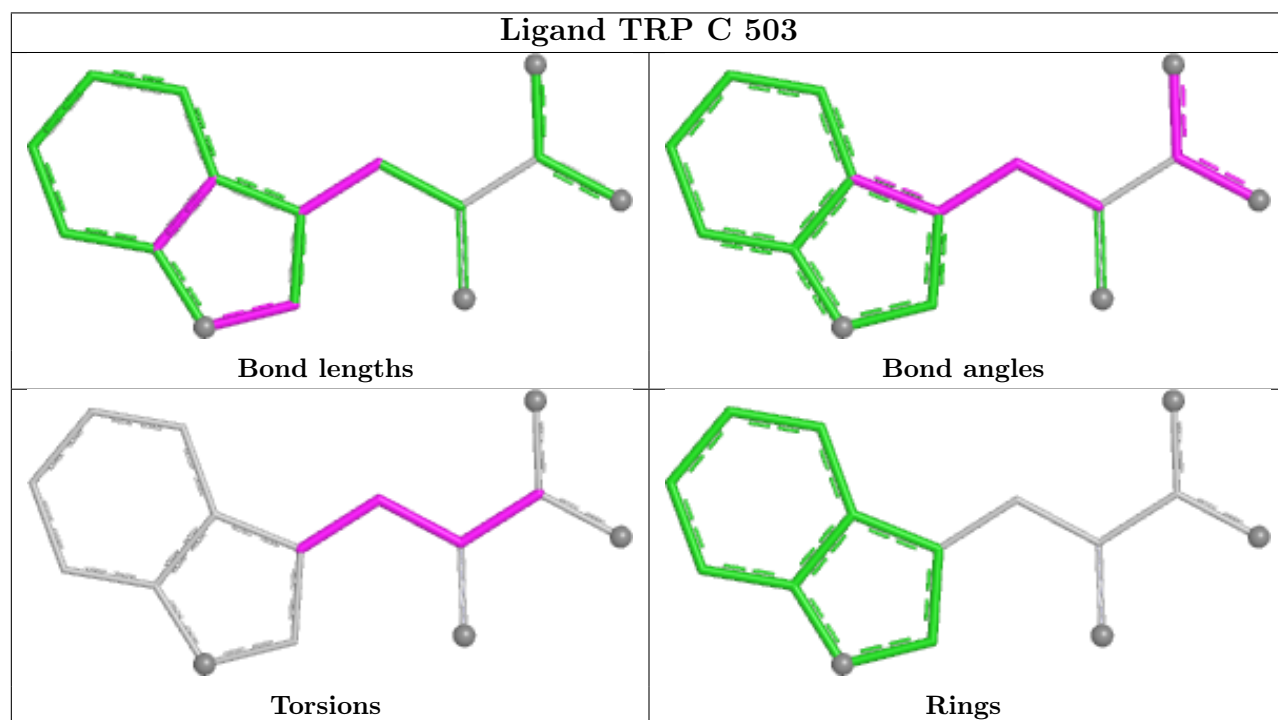
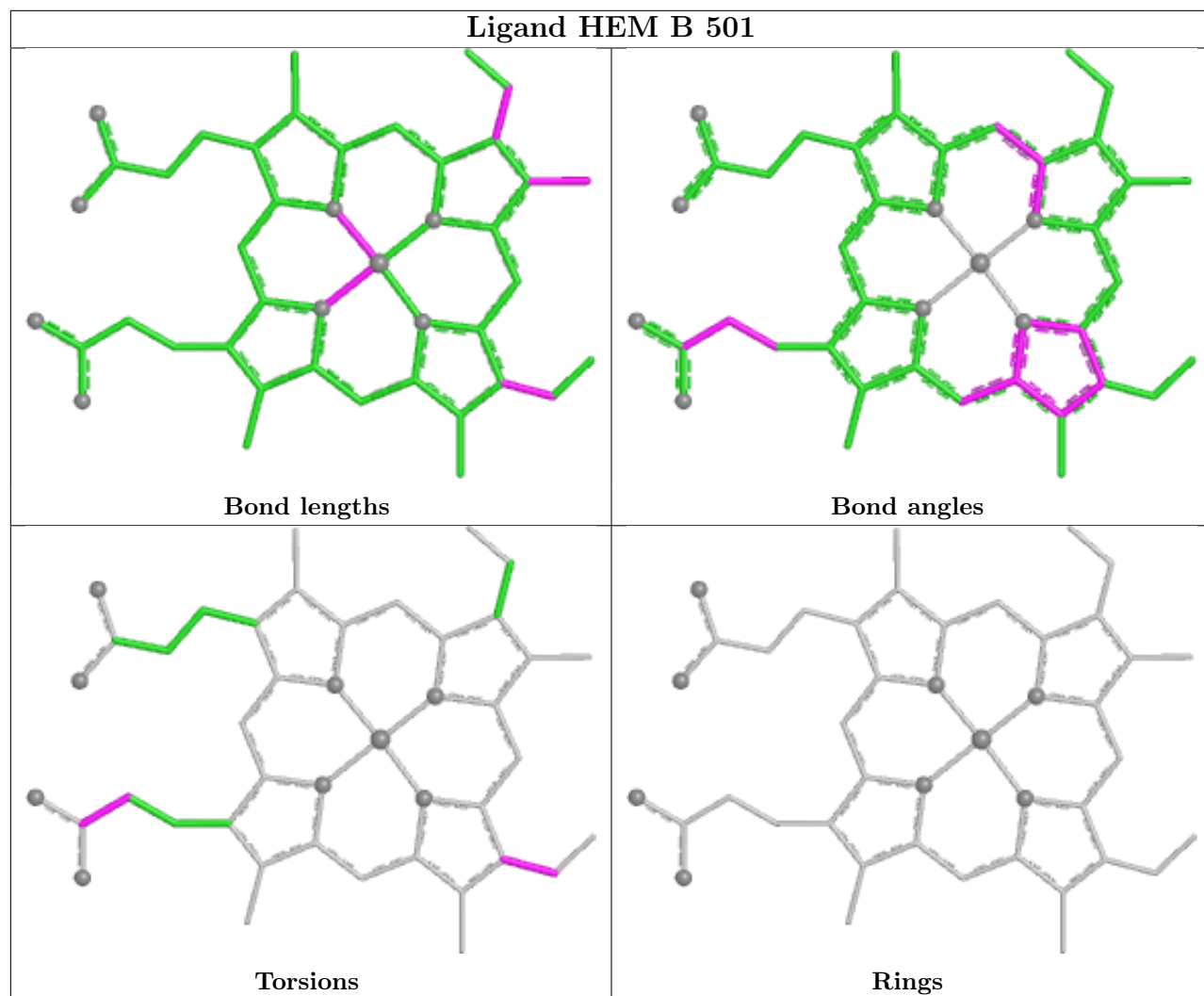
Ligand TRP D 505



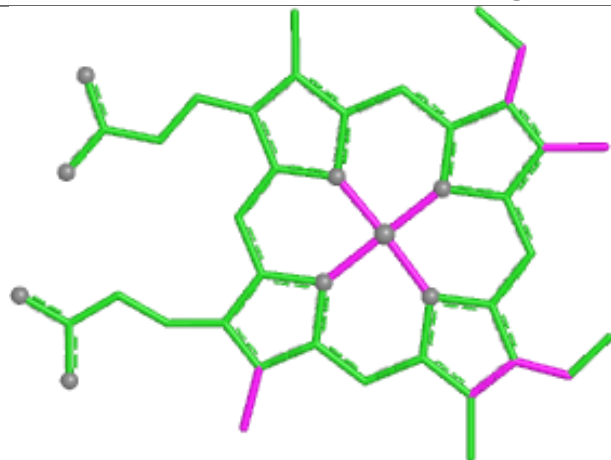
Ligand HEM D 501



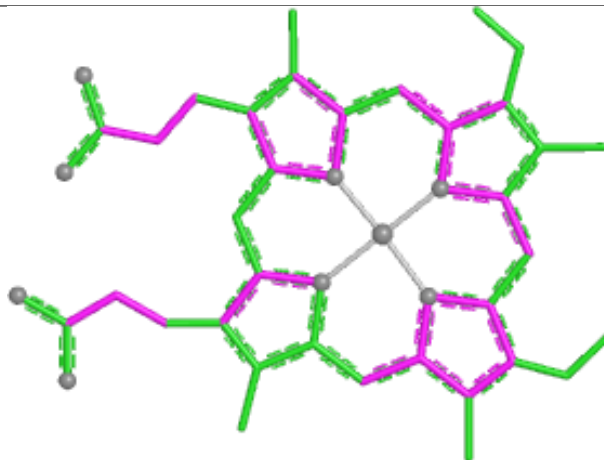




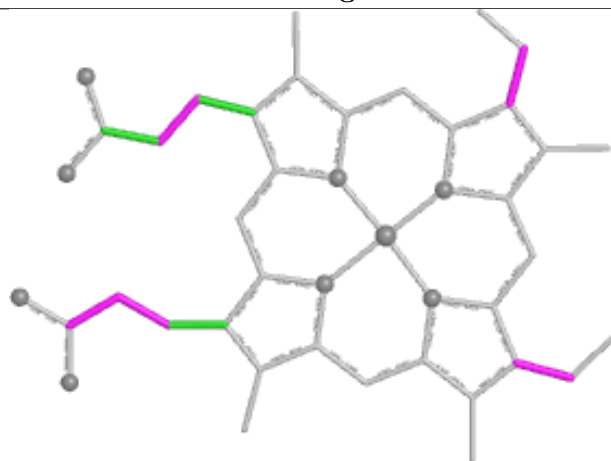
Ligand HEM A 501



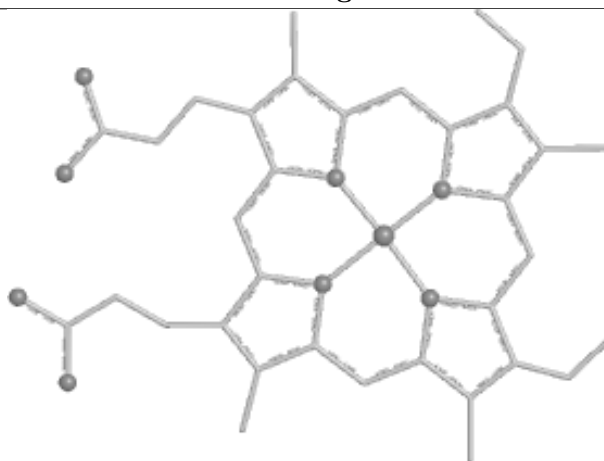
Bond lengths



Bond angles

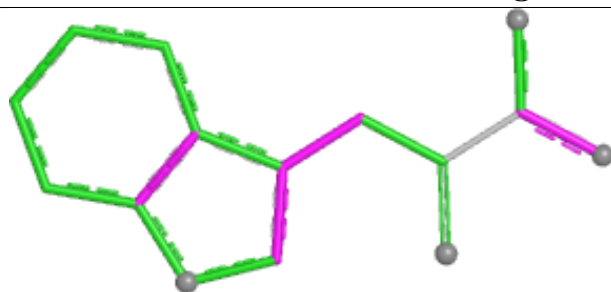


Torsions

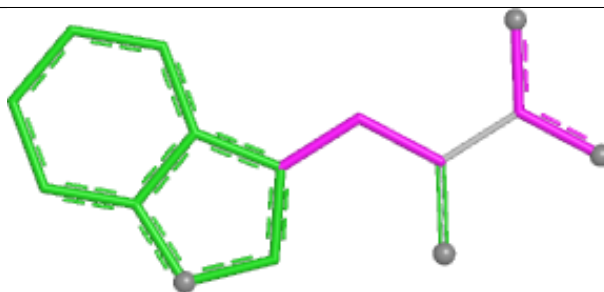


Rings

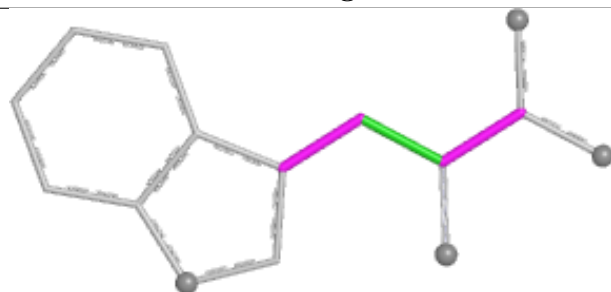
Ligand TRP D 504



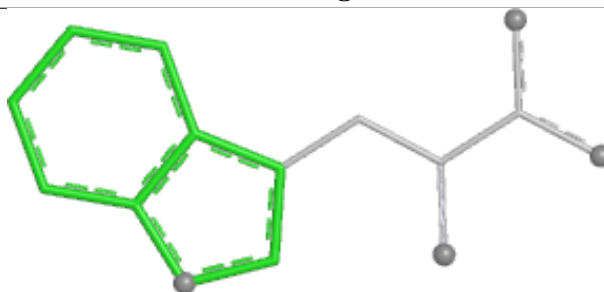
Bond lengths



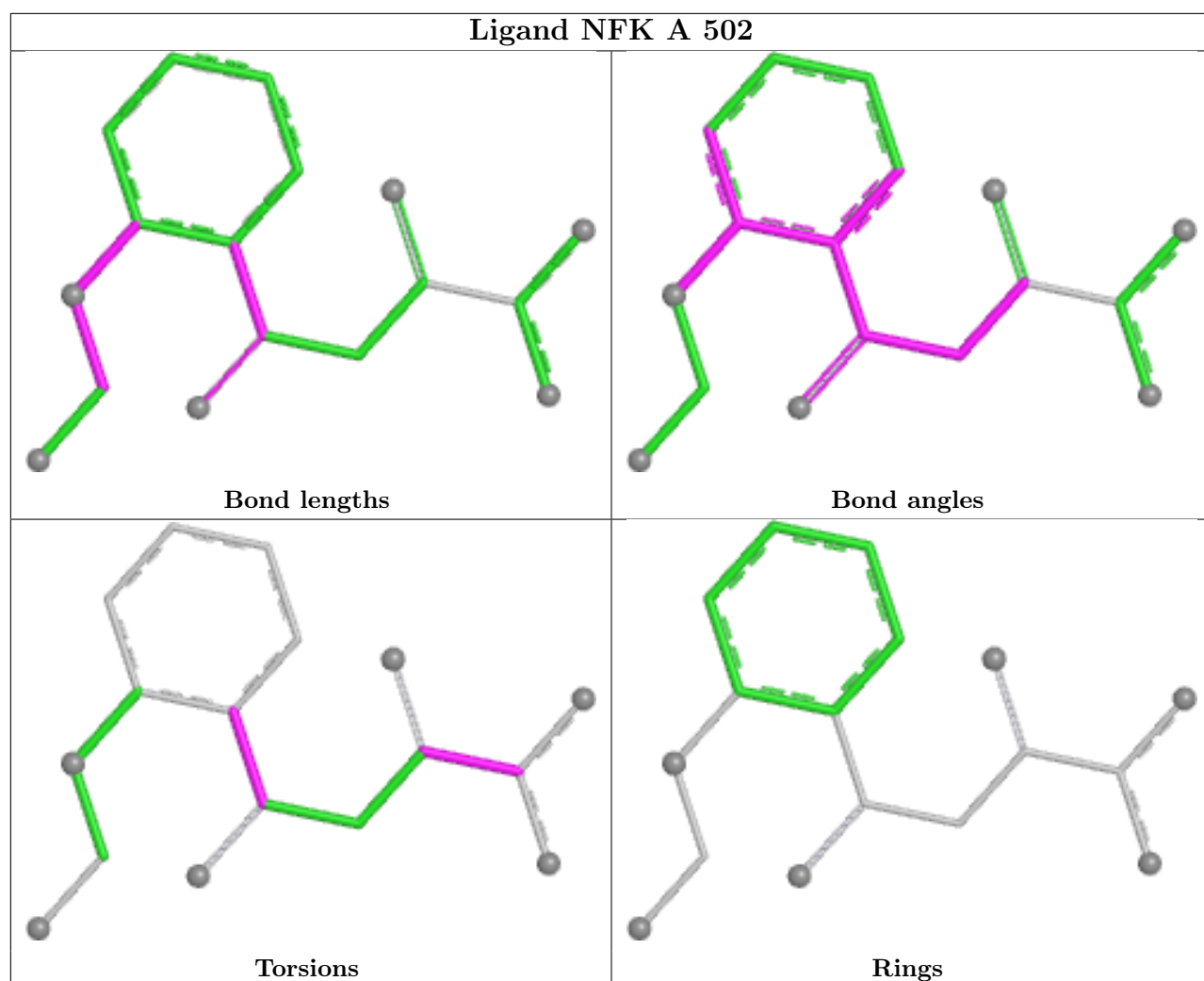
Bond angles

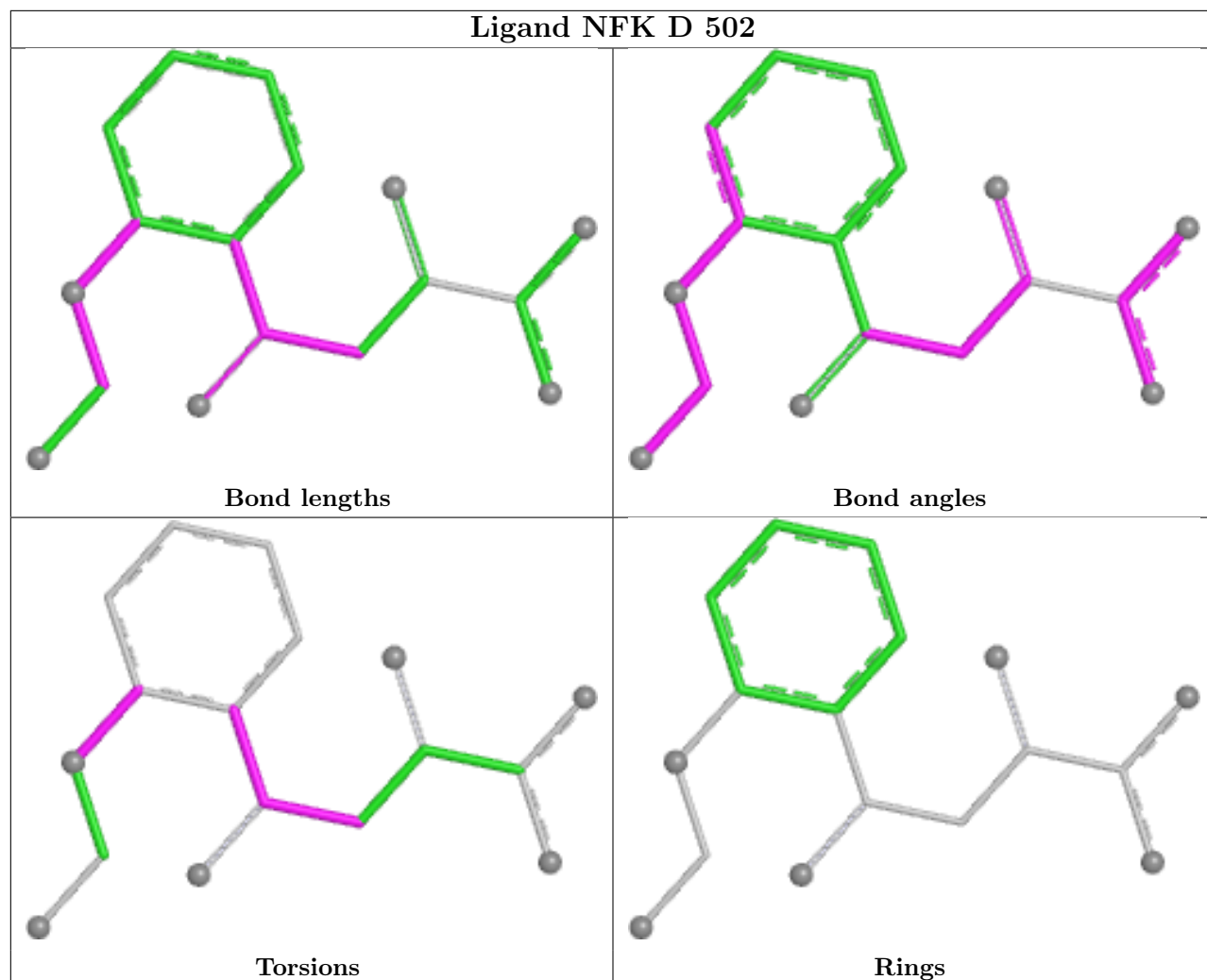


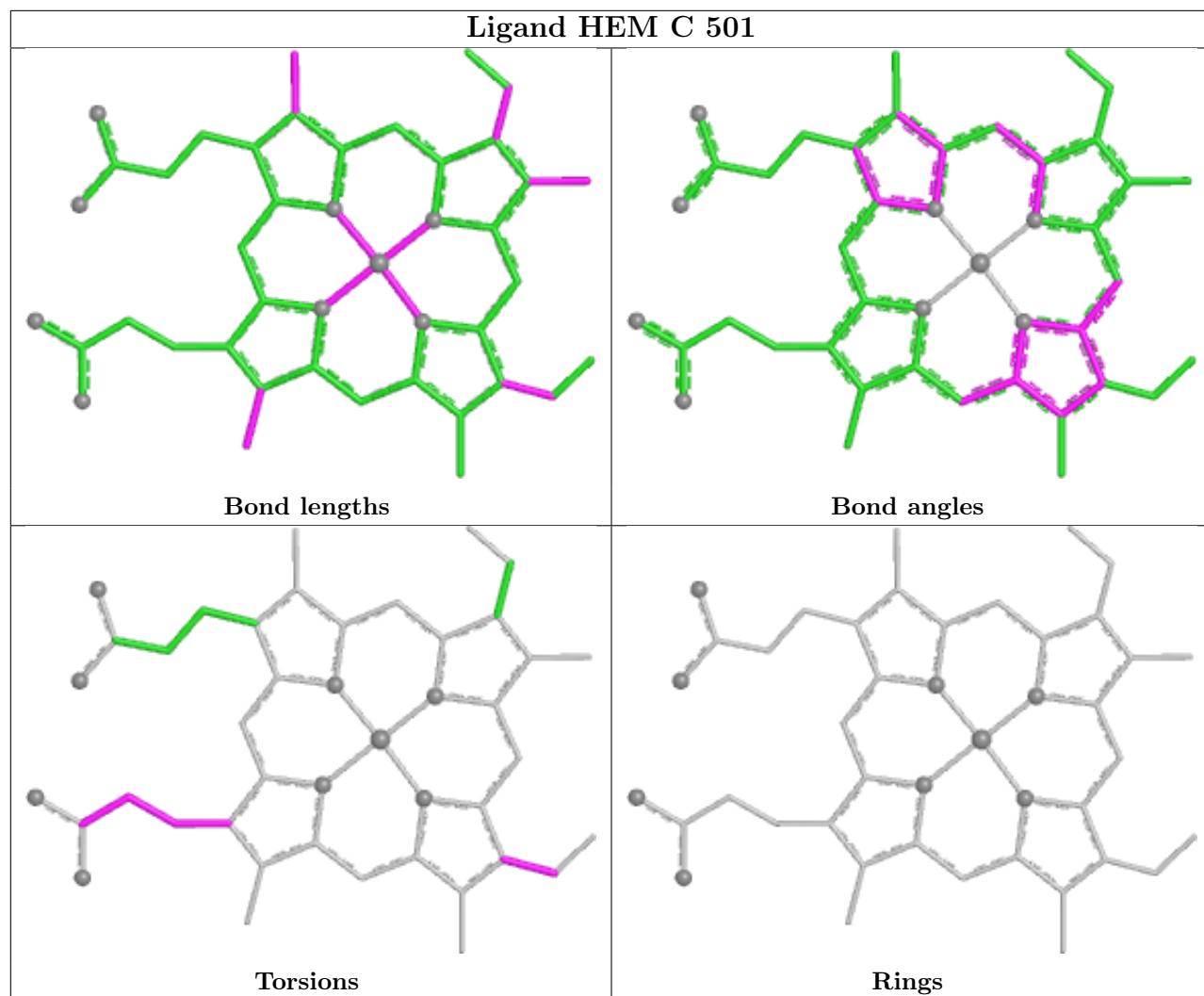
Torsions

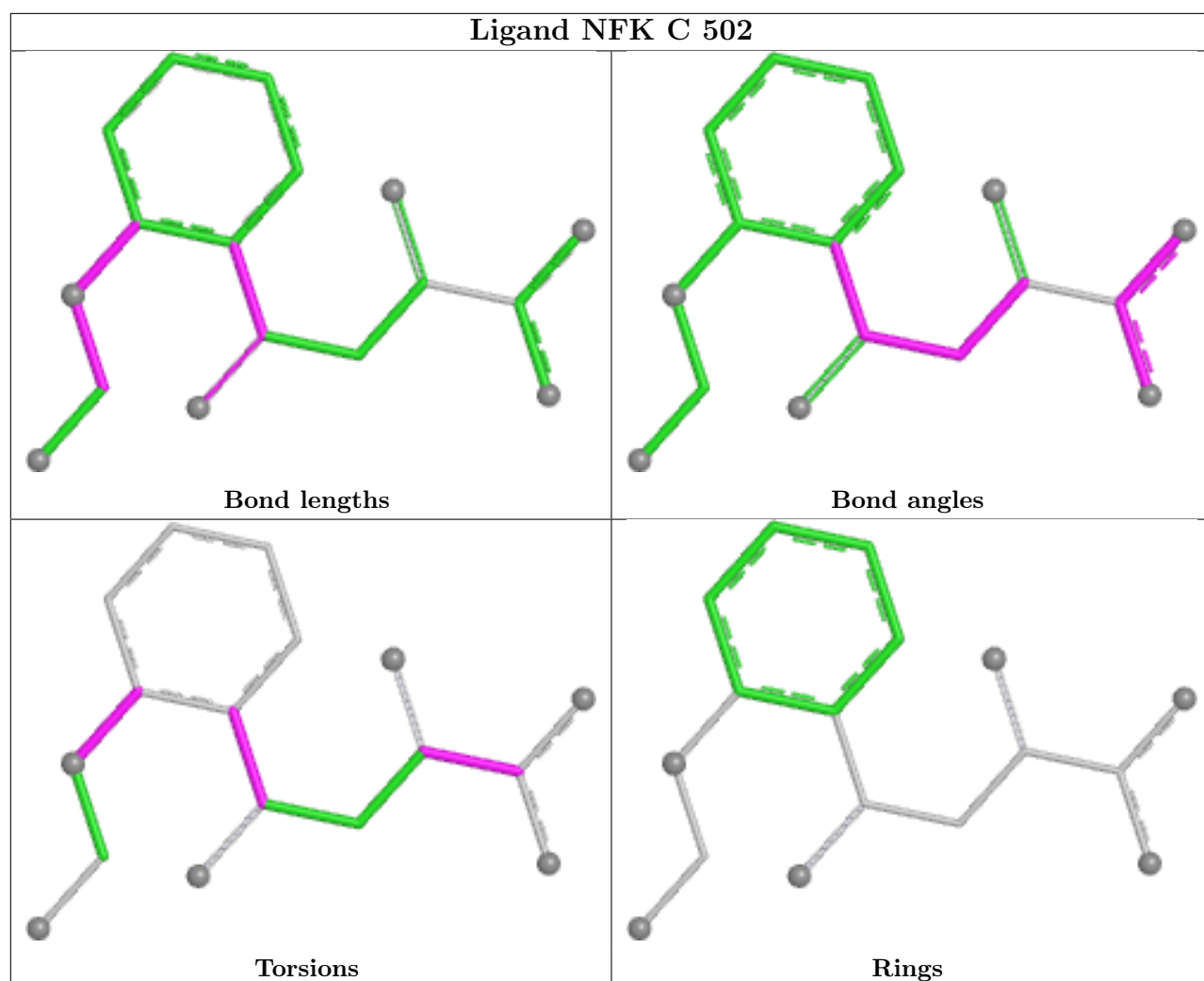


Rings









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	370/405 (91%)	0.05	9 (2%) 59 55	37, 56, 82, 106	0
1	B	375/405 (92%)	0.11	17 (4%) 38 33	37, 56, 89, 118	0
1	C	374/405 (92%)	0.08	13 (3%) 47 42	28, 55, 83, 112	1 (0%)
1	D	375/405 (92%)	0.16	16 (4%) 40 35	38, 58, 86, 122	0
All	All	1494/1620 (92%)	0.10	55 (3%) 45 40	28, 56, 86, 122	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	283	ALA	5.7
1	C	263	SER	4.6
1	B	262	GLY	4.3
1	A	282	THR	4.2
1	B	283	ALA	4.2
1	A	14	ALA	3.9
1	B	282	THR	3.7
1	A	283	ALA	3.6
1	D	282	THR	3.2
1	D	284	GLY	3.2
1	C	284	GLY	3.1
1	C	283	ALA	3.0
1	B	281	GLN	3.0
1	A	356	ILE	3.0
1	C	189	GLN	3.0
1	B	13	ALA	2.9
1	D	378	GLY	2.8
1	D	320	VAL	2.8
1	D	15	TYR	2.7
1	C	262	GLY	2.7
1	B	184	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	385	MET	2.7
1	D	265	GLY	2.6
1	A	281	GLN	2.6
1	B	285	GLY	2.5
1	B	16	HIS	2.4
1	C	282	THR	2.4
1	B	385	MET	2.4
1	A	382	THR	2.4
1	C	208[A]	GLU	2.4
1	D	382	THR	2.3
1	D	96	HIS	2.3
1	D	285	GLY	2.3
1	B	189	GLN	2.2
1	C	401	LYS	2.2
1	D	187	ALA	2.2
1	B	382	THR	2.2
1	C	383	ASP	2.2
1	D	379	THR	2.2
1	B	295	MET	2.1
1	C	264	ALA	2.1
1	C	379	THR	2.1
1	B	263	SER	2.1
1	B	190	MET	2.1
1	D	385	MET	2.1
1	C	14	ALA	2.1
1	A	265	GLY	2.1
1	C	321	LEU	2.1
1	A	381	GLY	2.1
1	D	380	GLY	2.1
1	B	379	THR	2.0
1	B	264	ALA	2.0
1	D	13	ALA	2.0
1	D	264	ALA	2.0
1	B	284	GLY	2.0

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

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

6.3 Carbohydrates [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.

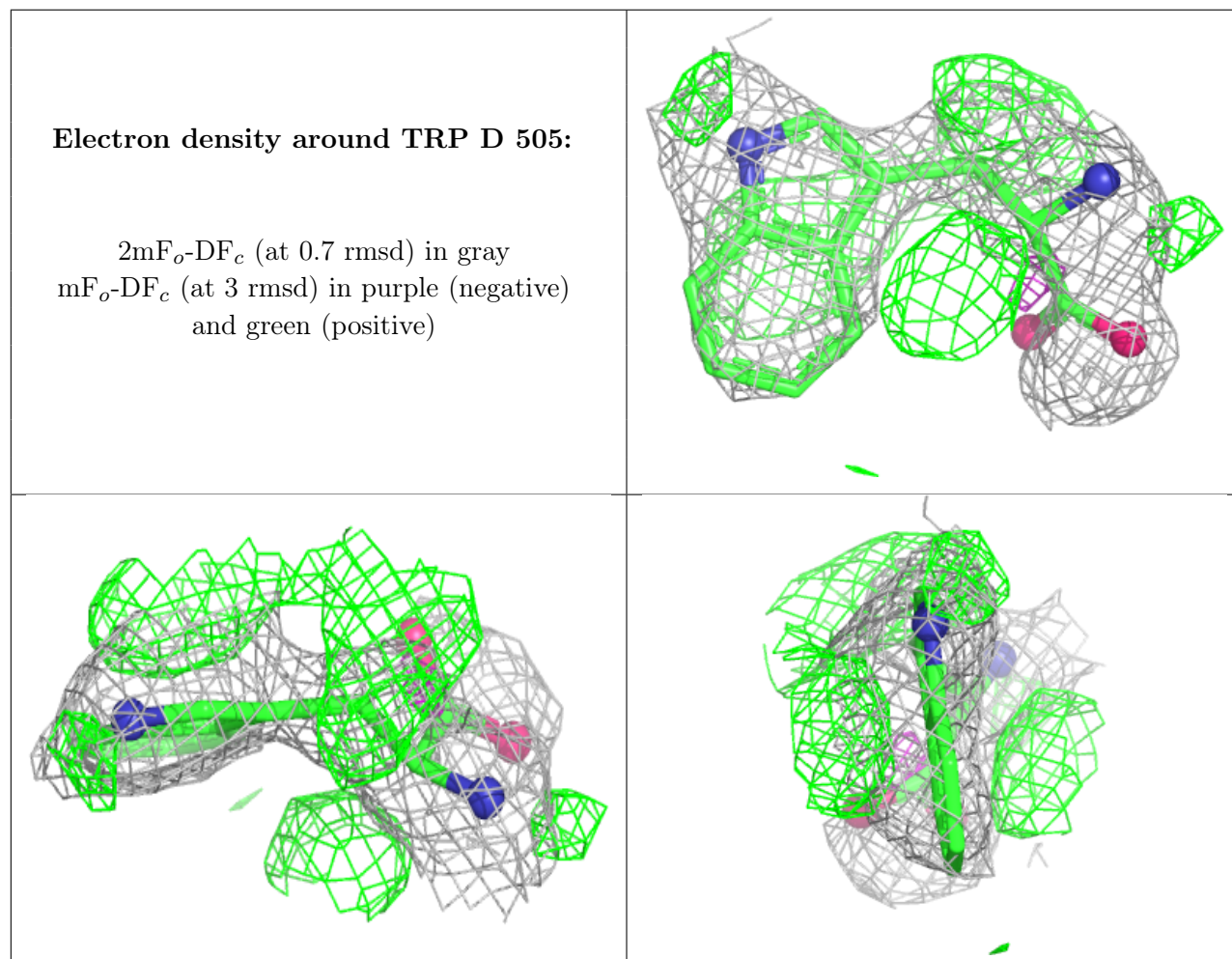
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TRP	D	505	15/15	0.67	0.24	46,54,61,64	15
4	PO4	C	504	5/5	0.72	0.15	88,89,100,114	0
3	NFK	D	502	17/17	0.73	0.22	47,59,68,69	17
5	GOL	A	506	6/6	0.75	0.18	65,66,67,78	6
5	GOL	C	510	6/6	0.76	0.16	74,81,82,85	0
3	NFK	A	502	17/17	0.76	0.24	57,63,70,72	17
5	GOL	D	507	6/6	0.78	0.21	62,72,78,80	0
6	OXY	B	508	2/2	0.78	0.13	74,74,74,78	0
4	PO4	A	503	5/5	0.78	0.13	53,54,63,63	5
7	TRP	D	504	15/15	0.79	0.20	54,60,62,64	15
5	GOL	A	504	6/6	0.80	0.23	60,62,67,71	0
3	NFK	C	502	17/17	0.81	0.15	61,71,76,76	17
5	GOL	D	506	6/6	0.81	0.13	57,61,63,65	0
5	GOL	A	508	6/6	0.81	0.20	63,66,70,70	0
5	GOL	C	511	6/6	0.82	0.15	50,59,62,64	0
3	NFK	D	503	17/17	0.82	0.15	60,73,80,85	17
8	CL	D	508	1/1	0.82	0.16	96,96,96,96	0
5	GOL	C	507	6/6	0.83	0.17	58,63,66,69	0
6	OXY	D	509	2/2	0.83	0.15	74,74,74,86	0
7	TRP	C	503	15/15	0.83	0.17	63,73,77,78	15
5	GOL	C	505	6/6	0.84	0.15	51,58,60,62	0
5	GOL	B	507	6/6	0.85	0.12	56,60,64,65	6
5	GOL	C	508	6/6	0.86	0.14	60,62,68,71	0
5	GOL	C	509	6/6	0.87	0.13	64,67,72,77	0
8	CL	C	512	1/1	0.88	0.14	105,105,105,105	0
5	GOL	A	507	6/6	0.88	0.10	60,63,70,77	0
6	OXY	A	510	2/2	0.90	0.11	74,74,74,75	0
5	GOL	B	506	6/6	0.90	0.12	56,58,58,71	6
5	GOL	C	506	6/6	0.90	0.09	61,66,68,77	0
5	GOL	B	505	6/6	0.90	0.13	64,66,70,75	0
5	GOL	A	505	6/6	0.91	0.12	51,56,57,60	0
5	GOL	B	502	6/6	0.91	0.13	50,57,61,63	0

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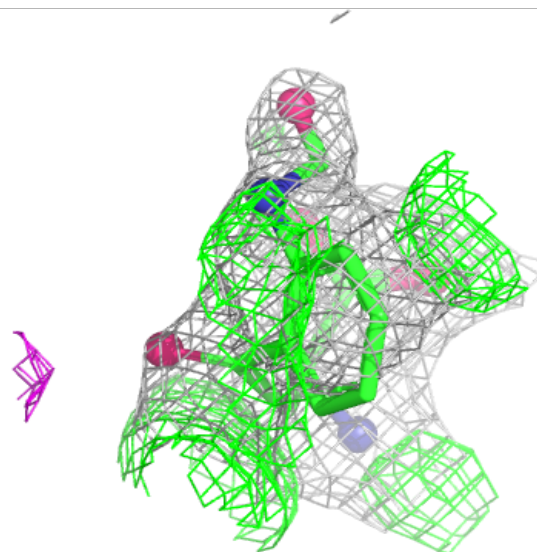
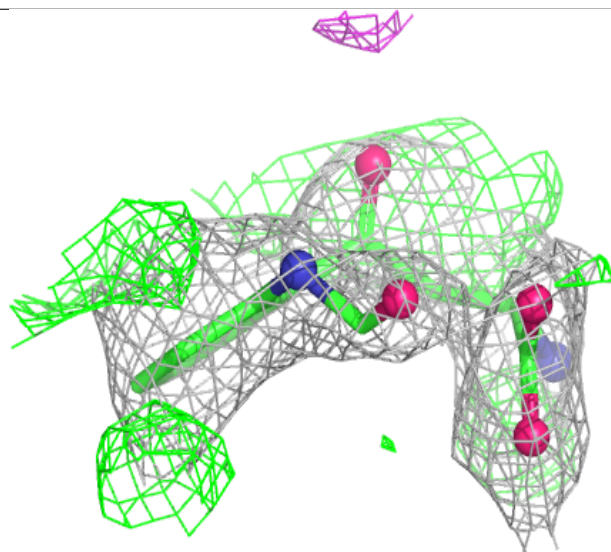
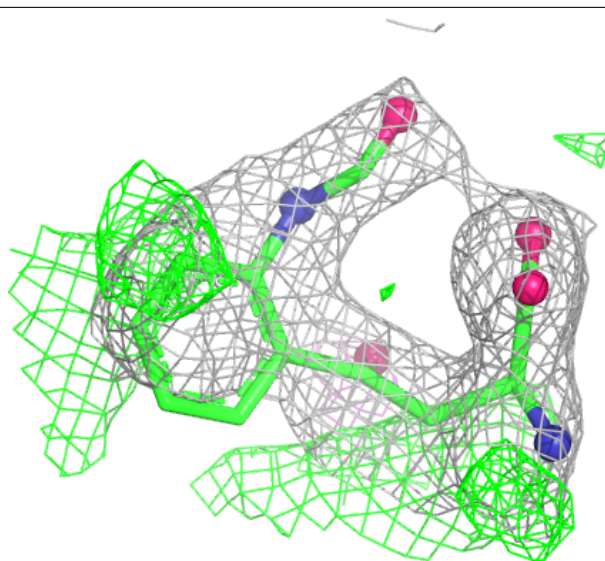
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	509	6/6	0.93	0.11	59,62,67,68	0
2	HEM	B	501	43/43	0.93	0.12	51,67,77,81	0
5	GOL	B	503	6/6	0.94	0.12	54,57,58,63	0
2	HEM	D	501	43/43	0.94	0.12	55,66,78,88	0
2	HEM	C	501	43/43	0.94	0.12	49,63,74,79	0
2	HEM	A	501	43/43	0.95	0.11	50,64,77,83	0
5	GOL	B	504	6/6	0.95	0.09	55,58,60,61	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.



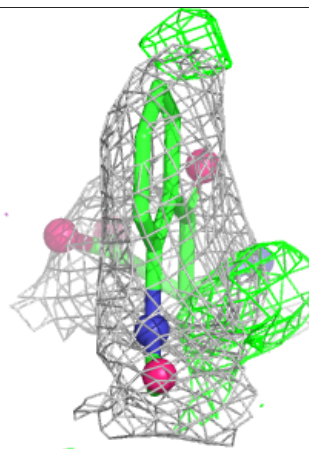
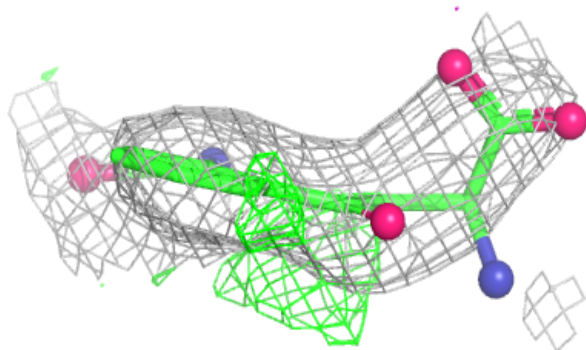
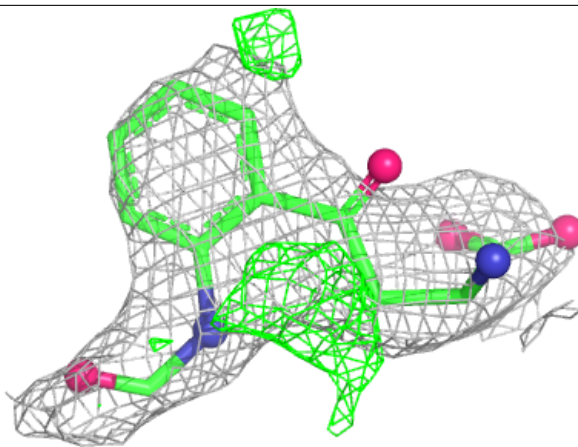
Electron density around NFK D 502:

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

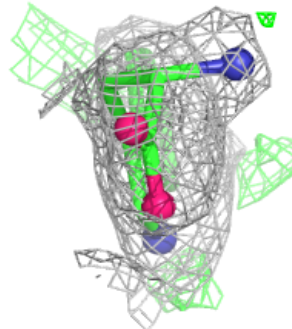
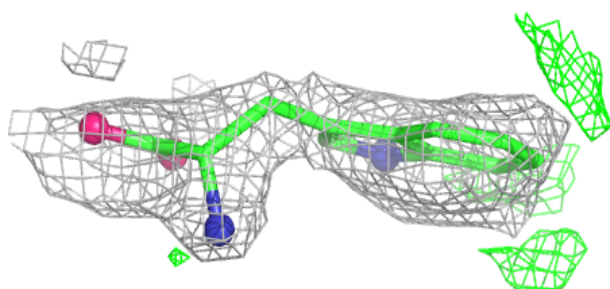
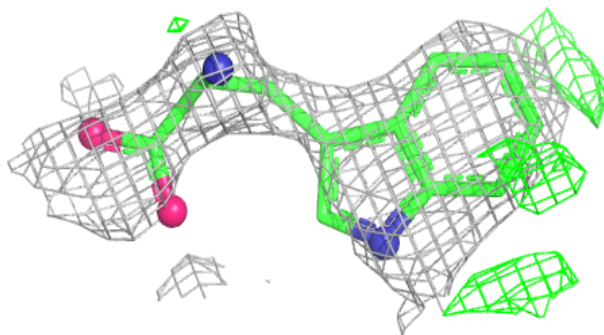


Electron density around NFK A 502:

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

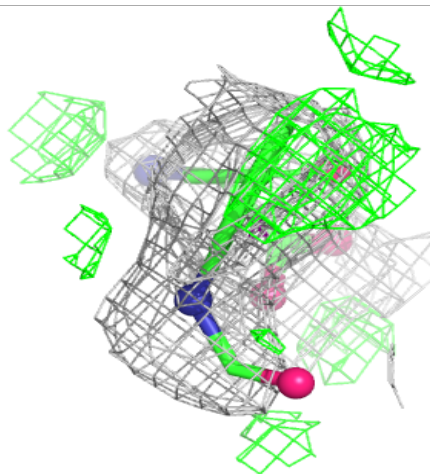
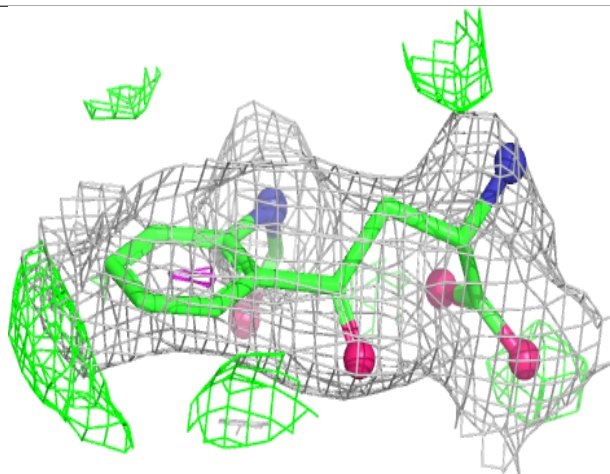
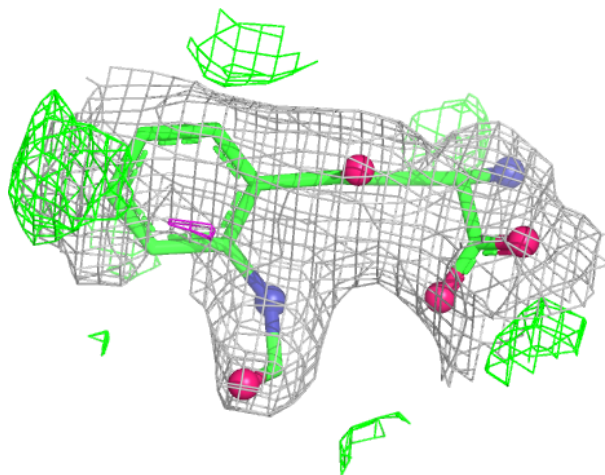
**Electron density around TRP D 504:**

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



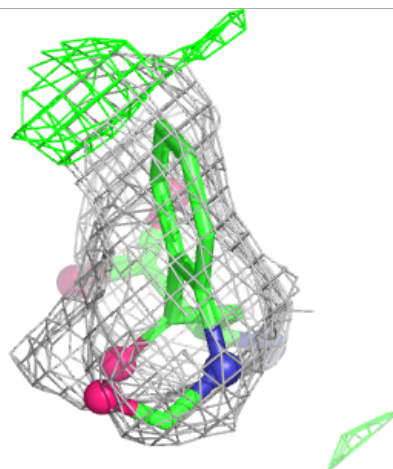
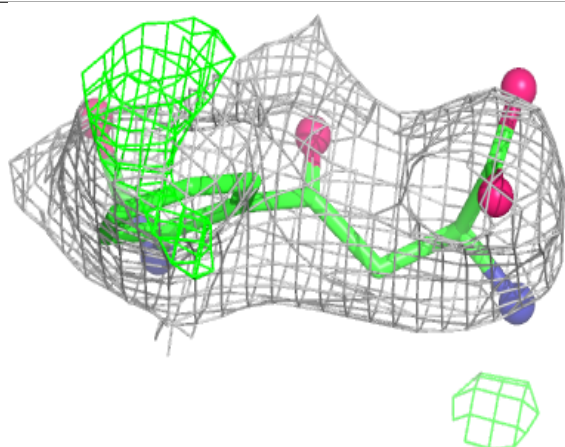
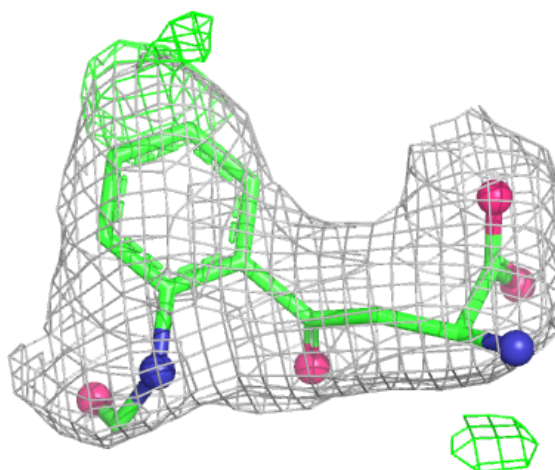
Electron density around NFK C 502:

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



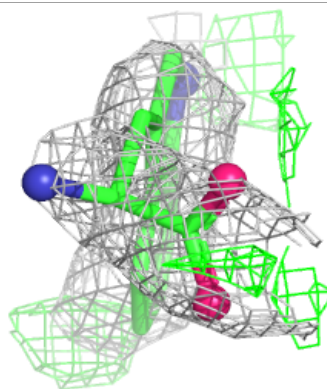
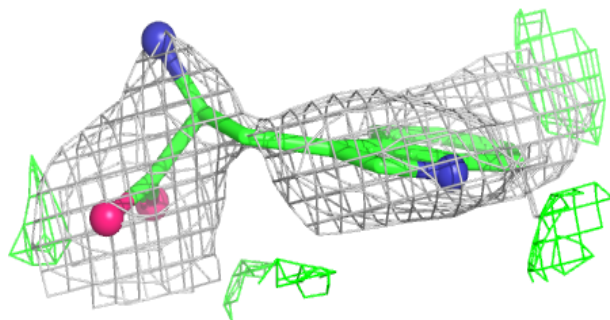
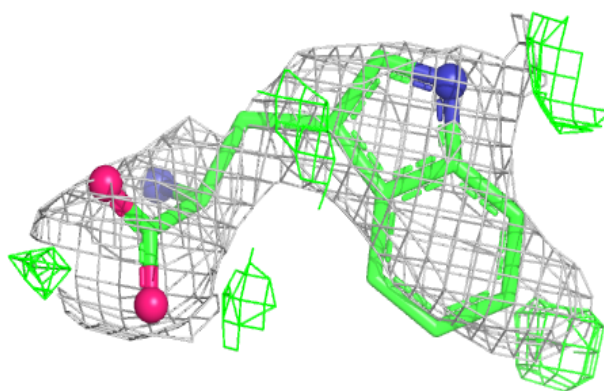
Electron density around NFK D 503:

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



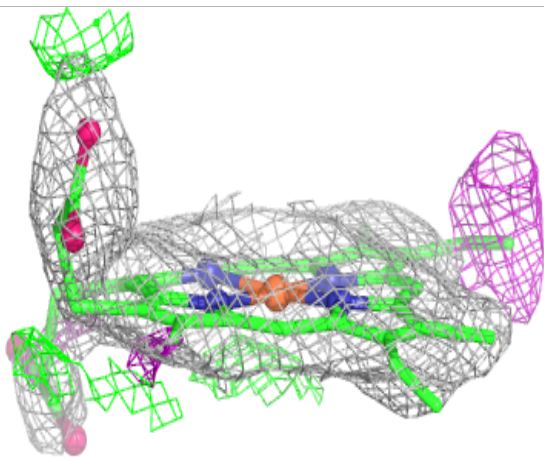
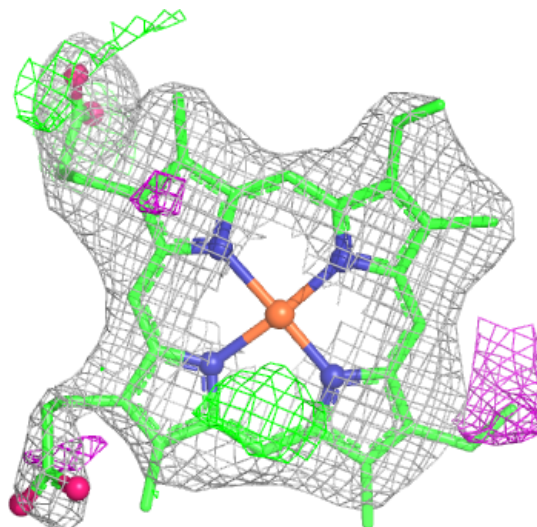
Electron density around TRP C 503:

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



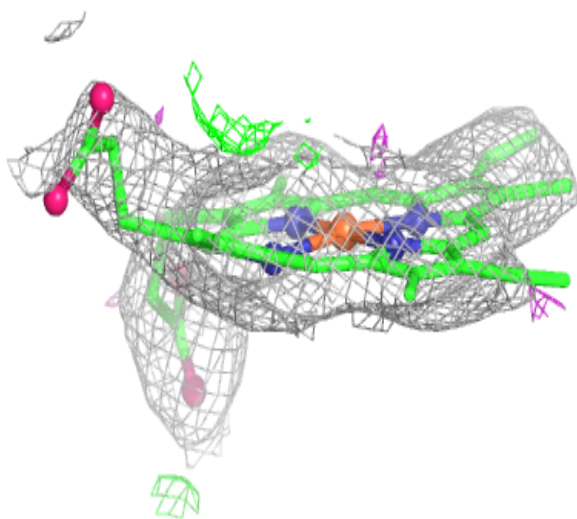
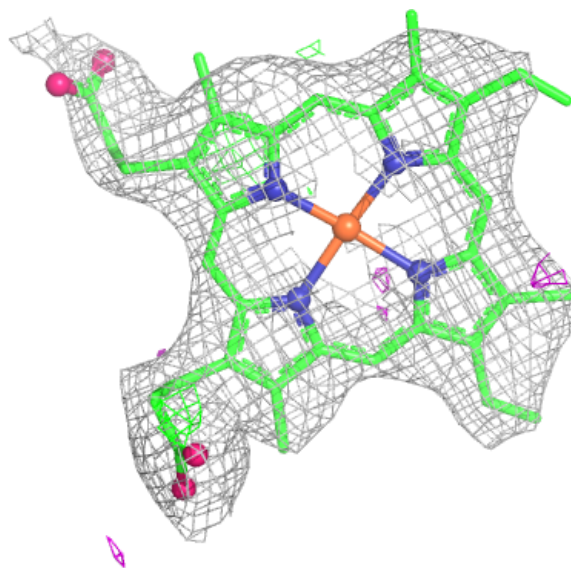
Electron density around HEM B 501:

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



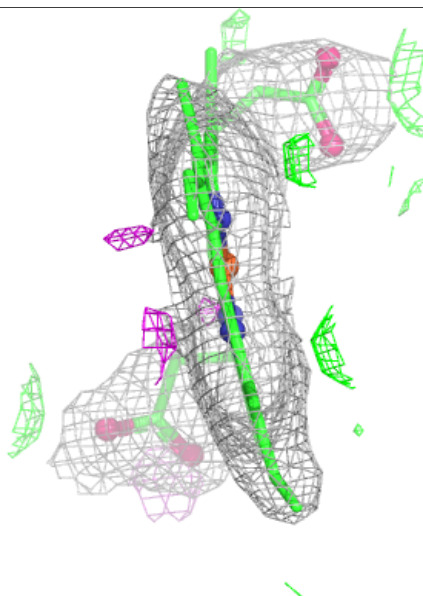
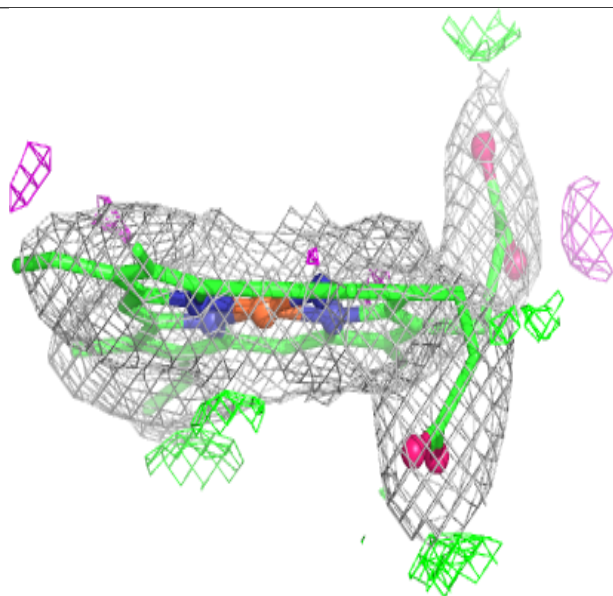
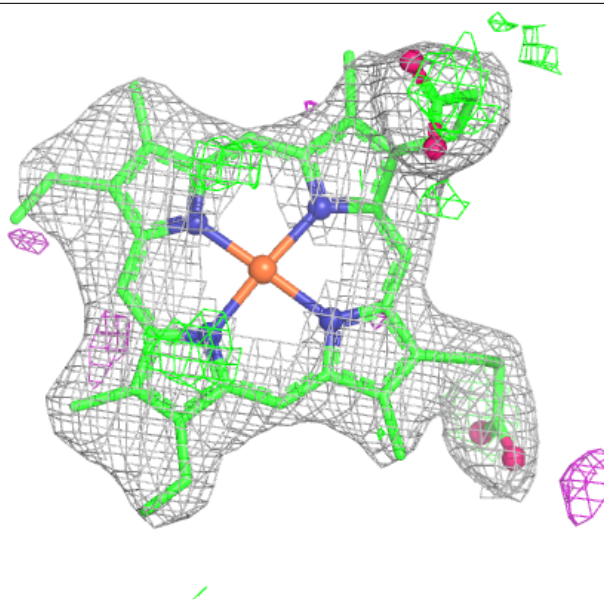
Electron density around HEM D 501:

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



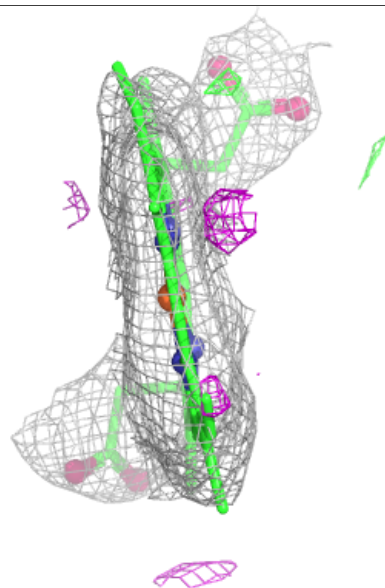
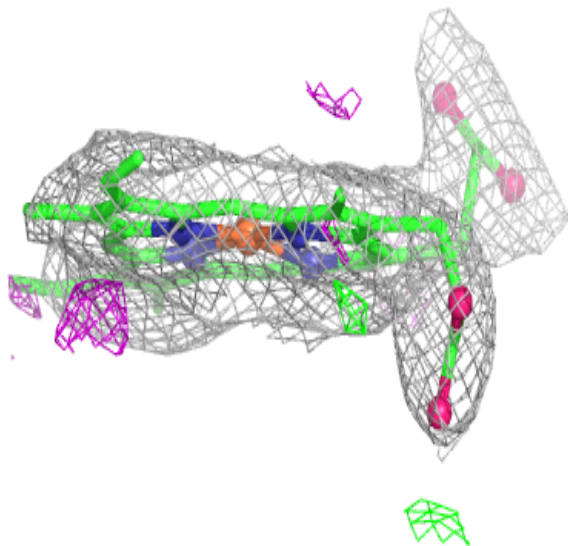
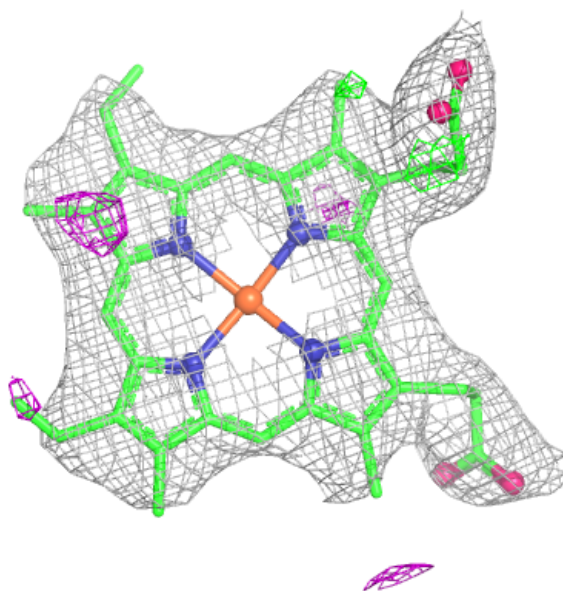
Electron density around HEM C 501:

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



Electron density around HEM A 501:

$2mF_o-DF_c$ (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.