



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 PM UTC

PDB ID : 7Z2L / pdb_00007z2l
Title : Crystal structure of L-Kynurenine in the active site of human Indoleamine-2,3-dioxygenase 1 (hIDO1)
Authors : Mirgaux, M.; Wouters, J.
Deposited on : 2022-02-28
Resolution : 2.56 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

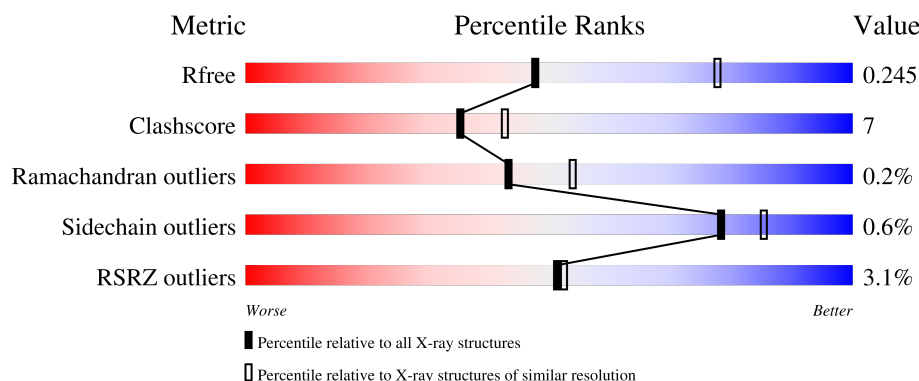
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	 2% 78% 13% 9%
1	B	405	 5% 78% 16% 6%
1	C	405	 2% 78% 14% 8%
1	D	405	 2% 80% 12% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13073 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	1	0
			2937	1888	500	531	18			
1	B	381	Total	C	N	O	S	0	3	0
			3012	1932	514	549	17			
1	C	372	Total	C	N	O	S	0	0	0
			2941	1891	501	532	17			
1	D	373	Total	C	N	O	S	0	0	0
			2946	1893	502	534	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

Continued on next page...

Continued from previous page...

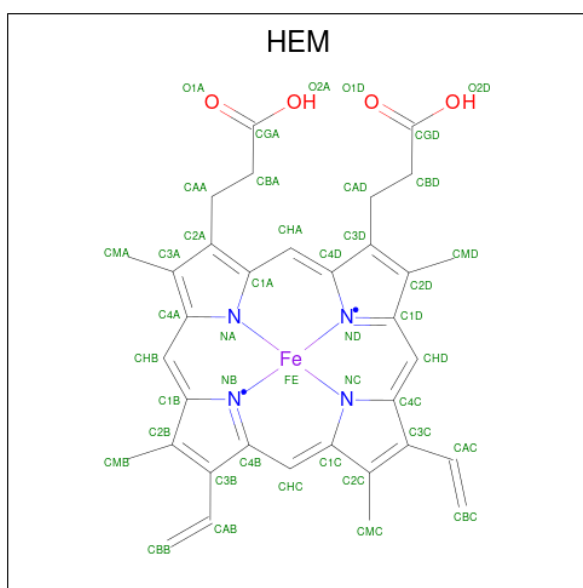
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	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

Continued on next page...

Continued from previous page...

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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



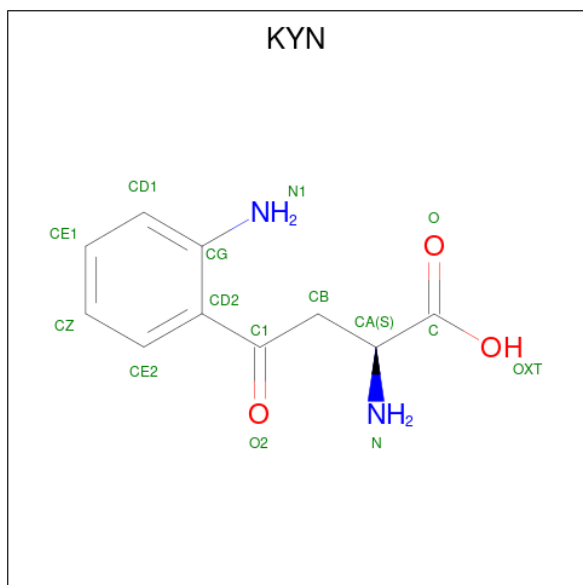
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

Continued on next page...

Continued from previous page...

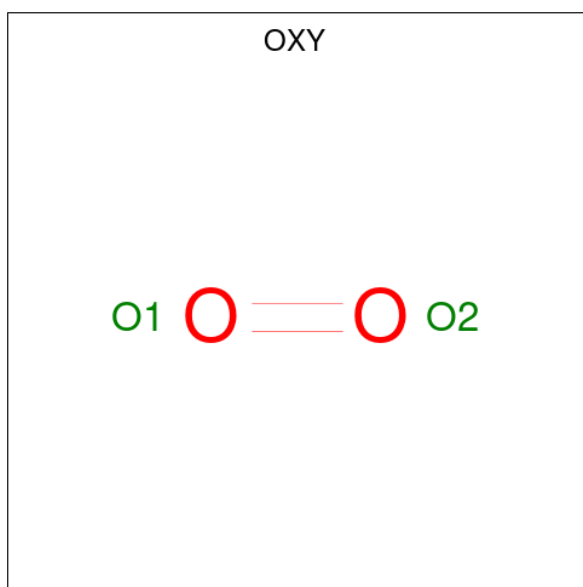
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is (2S)-2-amino-4-(2-aminophenyl)-4-oxobutanoic acid (CCD ID: KYN) (formula: $C_{10}H_{12}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	10	2	3		
4	B	1	Total	C	N	O	0	1
			22	16	3	3		
4	B	1	Total	C	N	O	0	0
			15	10	2	3		
4	B	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 2 2	0	1
5	C	1	Total O 2 2	0	0

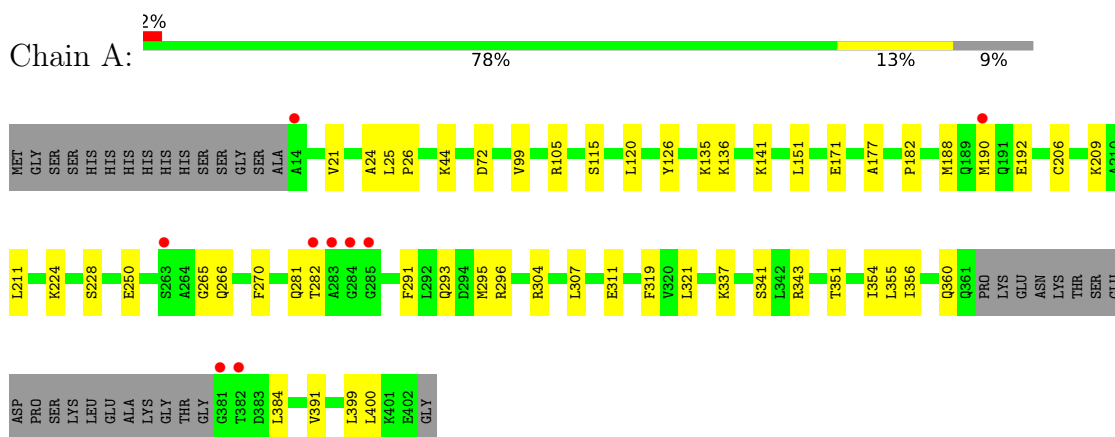
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	219	Total O 219 219	0	0
6	B	214	Total O 214 214	0	0
6	C	225	Total O 225 225	0	0
6	D	246	Total O 246 246	0	0

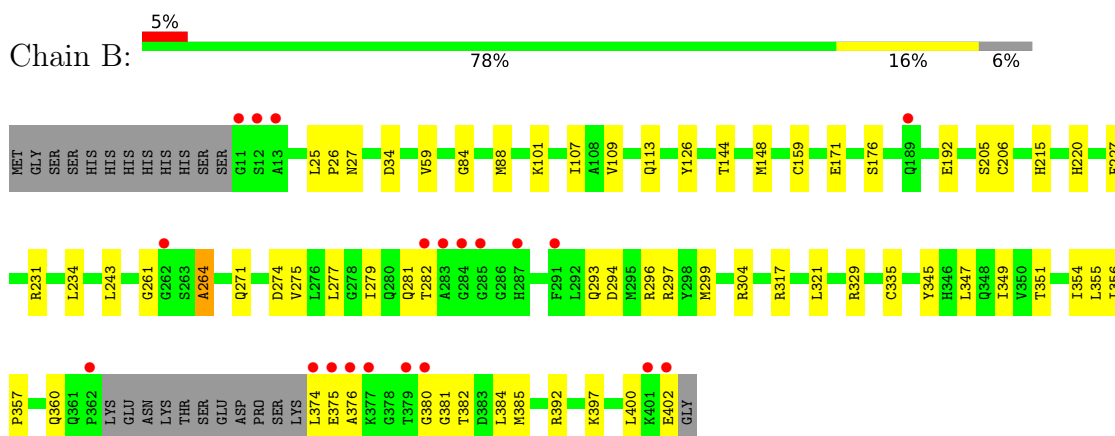
3 Residue-property plots [i](#)

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.

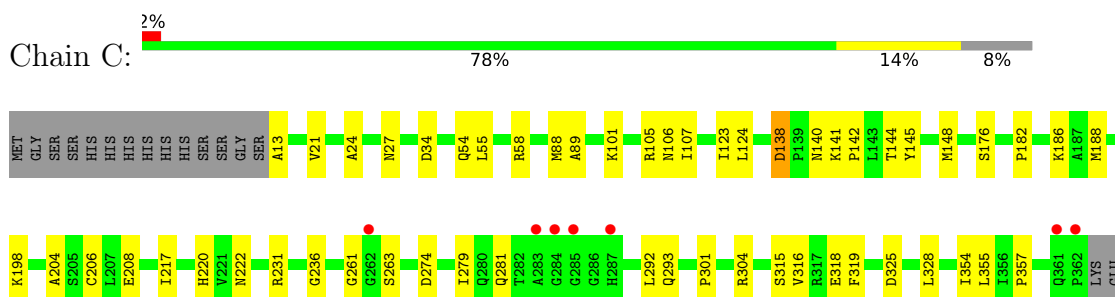
• Molecule 1: Indoleamine 2,3-dioxygenase 1

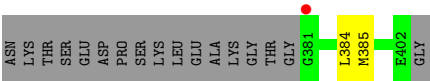


• Molecule 1: Indoleamine 2,3-dioxygenase 1

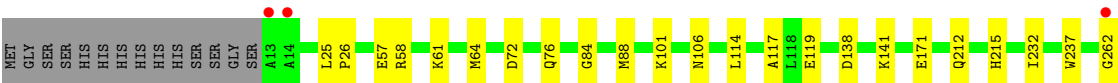
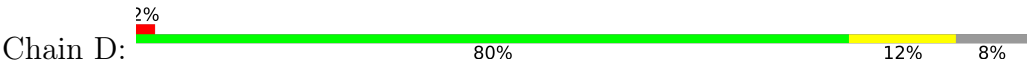


• Molecule 1: Indoleamine 2,3-dioxygenase 1





● 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	81.00Å 116.28Å 217.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 2.56 47.23 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.23-2.56) 99.2 (47.23-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.244 0.182 , 0.245	Depositor DCC
R_{free} test set	3331 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13073	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 46.95 % 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 1.0640e-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: KYN, OXY, HEM, 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	0.35	0/3005	0.52	0/4067
1	B	0.35	0/3081	0.53	0/4170
1	C	0.36	0/3010	0.54	0/4076
1	D	0.37	0/3015	0.54	1/4081 (0.0%)
All	All	0.36	0/12111	0.53	1/16394 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	GLY	N-CA-C	-5.58	99.94	113.18

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	2937	0	2943	37	0
1	B	3012	0	3015	49	0
1	C	2941	0	2947	42	0
1	D	2946	0	2950	32	0
2	A	43	0	30	7	0
2	B	43	0	30	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	4	0
2	D	43	0	30	7	0
3	A	30	0	40	2	0
3	B	12	0	16	1	0
3	C	24	0	32	7	0
3	D	24	0	32	0	0
4	A	15	0	11	3	0
4	B	52	0	34	8	0
5	B	2	0	0	1	0
5	C	2	0	0	0	0
6	A	219	0	0	2	0
6	B	214	0	0	6	0
6	C	225	0	0	10	0
6	D	246	0	0	6	0
All	All	13073	0	12140	180	0

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

All (180) 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)
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.54	0.89
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.55	0.86
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.56	0.86
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.58	0.85
1:D:354:ILE:HG13	2:D:501:HEM:HBC1	1.65	0.78
2:B:501:HEM:HBC2	2:B:501:HEM:HHH	1.67	0.75
1:C:354:ILE:HG13	2:C:501:HEM:HBC1	1.70	0.74
1:D:212:GLN:HA	1:D:215:HIS:HD2	1.51	0.74
1:C:186:LYS:NZ	6:C:601:HOH:O	2.22	0.72
1:D:57:GLU:HG2	1:D:61:LYS:HE3	1.72	0.72
4:B:505:KYN:N	6:B:603:HOH:O	2.24	0.69
1:B:355:LEU:HD13	1:B:374:LEU:HB2	1.73	0.69
2:D:501:HEM:HBC2	2:D:501:HEM:HHH	1.75	0.68
1:C:315:SER:HB3	1:C:318:GLU:HB2	1.76	0.67
1:B:227:PHE:O	1:B:231:ARG:NH1	2.27	0.67
1:A:182:PRO:HG3	3:A:504:GOL:H32	1.79	0.65
1:B:126:TYR:CD1	1:B:264[B]:ALA:HA	2.33	0.64
1:D:265:GLY:HA2	2:D:501:HEM:C2A	2.31	0.64
1:D:293:GLN:OE1	6:D:601:HOH:O	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HE2	1:A:224:LYS:H	1.63	0.63
1:A:296:ARG:O	1:A:304:ARG:HD2	1.98	0.63
1:C:236:GLY:N	1:C:261:GLY:HA3	2.14	0.63
1:C:355:LEU:HD11	1:C:385:MET:SD	2.39	0.62
1:B:271:GLN:HA	1:B:274:ASP:HB2	1.81	0.62
1:B:171:GLU:HG3	6:B:713:HOH:O	2.00	0.62
2:C:501:HEM:HBC2	2:C:501:HEM:HHD	1.82	0.61
4:B:503:KYN:O2	6:B:601:HOH:O	2.16	0.61
1:C:138:ASP:HB3	1:C:141:LYS:HD3	1.82	0.61
1:B:27:ASN:ND2	6:B:604:HOH:O	2.27	0.61
1:D:351:THR:HA	1:D:355:LEU:HB2	1.81	0.61
1:A:356:ILE:O	1:A:360:GLN:HG3	2.02	0.60
1:C:198:LYS:NZ	6:C:602:HOH:O	2.29	0.60
1:C:34:ASP:OD1	3:C:506:GOL:H11	2.02	0.59
1:B:261:GLY:H	3:B:504:GOL:H11	1.69	0.57
1:D:119:GLU:O	1:D:304:ARG:NH2	2.37	0.57
1:B:282:THR:OG1	1:B:293:GLN:HG2	2.04	0.57
1:A:171:GLU:HG3	6:A:691:HOH:O	2.05	0.57
1:A:282:THR:HG23	1:A:293:GLN:HE21	1.70	0.57
1:D:171:GLU:HG3	6:D:677:HOH:O	2.03	0.56
1:D:275:VAL:HG13	1:D:311:GLU:HG3	1.86	0.56
1:C:301:PRO:HB3	1:C:304:ARG:NH2	2.22	0.55
1:C:204:ALA:O	1:C:208:GLU:HG3	2.06	0.55
1:D:72:ASP:O	1:D:76:GLN:HG3	2.06	0.55
1:A:190:MET:HA	1:A:190:MET:HE2	1.88	0.54
1:D:389:LYS:NZ	6:D:606:HOH:O	2.39	0.54
1:D:101:LYS:HD3	6:D:783:HOH:O	2.06	0.54
1:C:182:PRO:HG3	3:C:505:GOL:H31	1.89	0.54
1:A:190:MET:HB3	1:A:192:GLU:HG2	1.90	0.54
1:C:138:ASP:OD1	1:C:140:ASN:N	2.29	0.54
1:C:220:HIS:HD1	3:C:502:GOL:HO1	1.55	0.53
4:B:505:KYN:HN1A	4:B:505:KYN:HB	1.72	0.53
1:A:321:LEU:HD21	1:A:400:LEU:HD22	1.90	0.53
1:D:350:VAL:HG11	1:D:384:LEU:HD21	1.90	0.53
1:B:357:PRO:HA	1:B:360:GLN:HG3	1.91	0.53
1:A:337:LYS:HG3	1:A:399:LEU:HD21	1.90	0.53
1:D:399:LEU:O	1:D:401:LYS:NZ	2.27	0.52
1:B:351:THR:O	1:B:356:ILE:HG12	2.10	0.52
1:B:376:ALA:HB3	1:B:380:GLY:HA3	1.90	0.52
1:B:385:MET:N	1:B:385:MET:HE2	2.25	0.52
1:C:274:ASP:OD2	1:C:281:GLN:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HB3	1:C:142:PRO:HD2	1.92	0.51
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	1.93	0.51
1:D:84:GLY:O	1:D:88:MET:HG2	2.11	0.50
1:A:188:MET:HG2	1:A:319:PHE:CD2	2.46	0.50
2:B:501:HEM:HMA1	2:B:501:HEM:O1A	2.12	0.50
1:D:138:ASP:HB3	1:D:141:LYS:HG3	1.93	0.50
1:B:25:LEU:HD12	1:B:26:PRO:HD2	1.93	0.50
1:A:44:LYS:HA	4:A:506:KYN:HZ	1.93	0.50
1:A:211:LEU:HD22	1:A:341:SER:HB3	1.94	0.50
1:B:264[B]:ALA:HB3	5:B:506[B]:OXY:O2	2.11	0.50
1:C:145:TYR:OH	3:C:502:GOL:H2	2.12	0.49
1:C:138:ASP:OD1	1:C:138:ASP:C	2.54	0.49
1:B:317:ARG:O	1:B:321:LEU:HB2	2.13	0.48
1:C:188:MET:HE3	1:C:319:PHE:HB2	1.95	0.48
1:D:262:GLY:HA2	1:D:266:GLN:NE2	2.28	0.48
3:A:503:GOL:O3	6:A:601:HOH:O	2.19	0.48
1:A:21:VAL:HB	1:A:24:ALA:HB3	1.94	0.48
1:B:296:ARG:O	1:B:304:ARG:HD3	2.13	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:CHD	2.41	0.48
1:B:329:ARG:NE	1:B:402:GLU:HB3	2.29	0.47
1:C:105:ARG:HD2	6:C:790:HOH:O	2.13	0.47
1:A:354:ILE:HG12	2:A:501:HEM:HBC1	1.97	0.46
1:C:293:GLN:HG3	6:C:711:HOH:O	2.16	0.46
1:B:234:LEU:HB2	4:B:502[B]:KYN:HD1	1.95	0.46
1:A:351:THR:HA	1:A:355:LEU:HB2	1.96	0.46
1:C:13:ALA:HB2	3:C:505:GOL:O1	2.16	0.46
1:D:262:GLY:HA2	1:D:266:GLN:HE22	1.81	0.46
1:C:21:VAL:HB	1:C:24:ALA:HB3	1.98	0.45
1:D:64:MET:HB2	1:D:106:ASN:OD1	2.17	0.45
1:C:325:ASP:HB3	1:C:328:LEU:HB2	1.98	0.45
1:D:76:GLN:HB3	1:D:114:LEU:HD11	1.97	0.45
1:C:88:MET:HE1	1:C:123:ILE:HG13	1.97	0.45
1:C:88:MET:HE3	1:C:124:LEU:H	1.81	0.45
1:A:25:LEU:HD12	1:A:26:PRO:HD2	1.98	0.45
1:D:25:LEU:HD12	1:D:26:PRO:HD2	1.99	0.45
1:B:321:LEU:HD12	1:B:321:LEU:HA	1.78	0.45
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.77	0.45
1:C:279:ILE:HG22	1:C:281:GLN:HG2	1.99	0.45
1:C:188:MET:SD	1:C:316:VAL:HG22	2.57	0.44
1:B:215:HIS:HD2	6:B:625:HOH:O	1.99	0.44
1:A:136:LYS:HE2	1:A:141:LYS:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LYS:HB2	1:B:397:LYS:HE2	1.81	0.44
2:C:501:HEM:HBC2	2:C:501:HEM:CHD	2.47	0.44
1:D:274:ASP:OD2	1:D:281:GLN:HG3	2.18	0.44
1:C:144:THR:O	1:C:148:MET:HG3	2.18	0.44
1:C:188:MET:HE3	1:C:319:PHE:CB	2.47	0.44
1:C:292:LEU:HD23	6:C:780:HOH:O	2.17	0.44
1:A:151:LEU:O	4:A:506:KYN:HE2	2.17	0.44
2:D:501:HEM:HBB2	2:D:501:HEM:CHC	2.36	0.44
1:B:192:GLU:OE2	6:B:602:HOH:O	2.21	0.44
1:D:271:GLN:HA	1:D:274:ASP:HB2	1.98	0.44
2:D:501:HEM:HBC2	2:D:501:HEM:CHD	2.41	0.44
1:B:274:ASP:OD2	1:B:281:GLN:HG3	2.18	0.44
1:A:135:LYS:HD3	4:A:506:KYN:O	2.17	0.44
1:D:356:ILE:HB	1:D:357:PRO:HD3	2.00	0.44
1:D:339:LEU:HD12	1:D:339:LEU:HA	1.77	0.43
1:C:222:ASN:ND2	6:C:605:HOH:O	2.41	0.43
1:A:265:GLY:HA2	2:A:501:HEM:C1A	2.54	0.43
1:A:384:LEU:HD11	2:A:501:HEM:HAD1	2.00	0.43
1:B:384:LEU:HD11	2:B:501:HEM:HAD1	2.00	0.43
1:C:176:SER:HB3	1:C:206:CYS:SG	2.58	0.43
1:B:296:ARG:HA	1:B:299:MET:HE3	2.01	0.43
1:C:27:ASN:ND2	6:C:614:HOH:O	2.51	0.43
1:C:54:GLN:O	1:C:58:ARG:HG2	2.19	0.43
1:C:101:LYS:HB2	1:C:101:LYS:HE2	1.46	0.43
1:B:392:ARG:HE	1:B:392:ARG:HB3	1.71	0.43
1:C:231:ARG:HD2	6:C:771:HOH:O	2.17	0.43
1:D:279:ILE:HD13	1:D:395:THR:HG23	2.01	0.43
1:B:321:LEU:HD13	1:B:400:LEU:HD22	2.01	0.42
1:B:109:VAL:O	1:B:113:GLN:HG3	2.20	0.42
1:C:55:LEU:HD22	1:C:89:ALA:HB1	2.01	0.42
1:A:115:SER:HB3	1:A:120:LEU:O	2.20	0.42
1:B:345:TYR:CE2	1:B:349:ILE:HD11	2.54	0.42
3:C:506:GOL:H32	6:C:766:HOH:O	2.19	0.42
1:D:291:PHE:CZ	1:D:295:MET:HE2	2.54	0.42
1:A:270:PHE:HB3	1:A:343:ARG:NH2	2.34	0.42
1:B:59:VAL:HG13	1:B:107:ILE:HG13	2.01	0.42
1:B:101:LYS:HG2	1:B:243:LEU:CD2	2.50	0.42
1:B:294:ASP:O	1:B:297:ARG:HB2	2.19	0.42
1:B:34:ASP:OD1	1:B:34:ASP:N	2.52	0.42
1:C:301:PRO:HB3	1:C:304:ARG:HH21	1.85	0.42
1:B:355:LEU:HD21	1:B:385:MET:HE3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:505:KYN:HD1	1:D:117:ALA:HB1	2.01	0.42
2:D:501:HEM:HHC	2:D:501:HEM:CBB	2.40	0.42
1:A:224:LYS:O	1:A:228:SER:HB2	2.20	0.42
1:A:281:GLN:NE2	1:A:391:VAL:HG13	2.35	0.42
1:A:291:PHE:CZ	2:A:501:HEM:HBD1	2.55	0.42
1:A:384:LEU:HD21	2:A:501:HEM:HMD2	2.01	0.41
1:B:271:GLN:O	1:B:275:VAL:HG23	2.20	0.41
1:B:354:ILE:HG12	2:B:501:HEM:CBC	2.50	0.41
1:A:209:LYS:HB3	1:A:209:LYS:HE2	1.84	0.41
1:B:356:ILE:HG12	1:B:356:ILE:H	1.74	0.41
1:B:400:LEU:O	1:B:402:GLU:HB2	2.20	0.41
1:A:72:ASP:OD1	1:A:72:ASP:N	2.54	0.41
1:A:295[B]:MET:HE2	1:A:295[B]:MET:HB2	1.77	0.41
1:B:144:THR:O	1:B:148:MET:HG3	2.20	0.41
1:B:159:CYS:SG	4:B:503:KYN:HB	2.60	0.41
1:B:374:LEU:HB3	1:B:375:GLU:H	1.64	0.41
1:A:188:MET:HG2	1:A:319:PHE:CG	2.56	0.41
1:B:176:SER:HB3	1:B:206:CYS:SG	2.61	0.41
1:B:220:HIS:HA	4:B:503:KYN:HE2	2.02	0.41
1:D:401:LYS:NZ	6:D:602:HOH:O	2.33	0.41
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.83	0.41
2:B:501:HEM:HBB2	2:B:501:HEM:CHC	2.35	0.41
1:A:126:TYR:HB2	1:A:266:GLN:HB2	2.02	0.41
1:B:84:GLY:O	1:B:88:MET:HG2	2.20	0.41
1:C:106:ASN:HB2	6:C:663:HOH:O	2.21	0.41
1:A:105:ARG:N	1:A:250:GLU:OE2	2.44	0.41
1:A:291:PHE:CE1	1:A:295[B]:MET:SD	3.14	0.41
1:A:307:LEU:O	1:A:311:GLU:HG3	2.21	0.41
1:B:277:LEU:HD11	1:B:335:CYS:HB3	2.03	0.40
1:C:354:ILE:C	1:C:357:PRO:HD2	2.46	0.40
1:D:58:ARG:HD2	6:D:604:HOH:O	2.20	0.40
1:D:296:ARG:HA	1:D:299:MET:HE3	2.02	0.40
1:C:384:LEU:HD23	1:C:385:MET:N	2.36	0.40
1:C:182:PRO:CG	3:C:505:GOL:H31	2.51	0.40
1:A:177:ALA:HB2	1:A:206:CYS:HB2	2.03	0.40
1:B:277:LEU:HB2	1:B:279:ILE:HD12	2.03	0.40
4:B:505:KYN:HD1	1:D:76:GLN:HE22	1.86	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	367/405 (91%)	352 (96%)	15 (4%)	0	100	100
1	B	380/405 (94%)	360 (95%)	17 (4%)	3 (1%)	16	22
1	C	368/405 (91%)	350 (95%)	17 (5%)	1 (0%)	36	44
1	D	369/405 (91%)	354 (96%)	15 (4%)	0	100	100
All	All	1484/1620 (92%)	1416 (95%)	64 (4%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	263	SER
1	B	264[A]	ALA
1	B	264[B]	ALA
1	B	381	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/346 (92%)	318 (100%)	1 (0%)	86	91
1	B	325/346 (94%)	323 (99%)	2 (1%)	78	85
1	C	319/346 (92%)	316 (99%)	3 (1%)	70	80
1	D	319/346 (92%)	317 (99%)	2 (1%)	78	85
All	All	1282/1384 (93%)	1274 (99%)	8 (1%)	78	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	B	205	SER
1	B	382	THR
1	C	107	ILE
1	C	138	ASP
1	C	217	ILE
1	D	232	ILE
1	D	237	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	76	GLN
1	A	96	HIS
1	A	242	GLN
1	A	293	GLN
1	A	386	ASN
1	B	29	GLN
1	B	216	GLN
1	C	29	GLN
1	C	63	ASN
1	C	69	HIS
1	C	216	GLN
1	D	27	ASN
1	D	73	HIS
1	D	96	HIS
1	D	216	GLN
1	D	220	HIS
1	D	287	HIS
1	D	348	GLN

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 ⓘ

26 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	$\# Z > 2$
3	GOL	B	504	-	5,5,5	1.23	0	5,5,5	0.74	0
3	GOL	C	503	-	5,5,5	1.18	0	5,5,5	0.88	0
3	GOL	C	502	-	5,5,5	1.06	0	5,5,5	0.85	0
5	OXY	C	504	-	1,1,1	0.32	0	-		
3	GOL	D	503	-	5,5,5	1.01	0	5,5,5	1.15	0
3	GOL	D	502	-	5,5,5	1.45	1 (20%)	5,5,5	0.95	0
2	HEM	A	501	1	50,50,50	1.68	8 (16%)	67,82,82	1.54	13 (19%)
5	OXY	B	506[B]	2	1,1,1	0.34	0	-		
3	GOL	A	505	-	5,5,5	0.97	0	5,5,5	1.17	0
3	GOL	C	506	-	5,5,5	1.05	0	5,5,5	1.34	1 (20%)
4	KYN	B	503	-	14,15,15	1.55	4 (28%)	15,20,20	1.31	2 (13%)
3	GOL	A	504	-	5,5,5	1.10	1 (20%)	5,5,5	1.18	0
3	GOL	B	507	-	5,5,5	0.93	0	5,5,5	1.11	0
4	KYN	B	505	-	14,15,15	1.38	3 (21%)	15,20,20	1.79	3 (20%)
2	HEM	B	501	5,1	50,50,50	1.72	6 (12%)	67,82,82	1.54	15 (22%)
2	HEM	C	501	1	50,50,50	1.56	7 (14%)	67,82,82	1.65	16 (23%)
3	GOL	D	504	-	5,5,5	1.22	0	5,5,5	0.85	0
4	KYN	B	502[A]	-	14,15,15	1.43	3 (21%)	15,20,20	1.05	1 (6%)
2	HEM	D	501	1	50,50,50	1.65	8 (16%)	67,82,82	1.70	15 (22%)
3	GOL	A	503	-	5,5,5	0.97	0	5,5,5	1.08	0
3	GOL	A	507	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	C	505	-	5,5,5	1.21	0	5,5,5	0.85	0
4	KYN	B	502[B]	-	14,15,15	1.40	3 (21%)	15,20,20	1.14	1 (6%)
3	GOL	A	502	-	5,5,5	0.97	0	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	505	-	5,5,5	0.97	0	5,5,5	1.11	1 (20%)
4	KYN	A	506	-	14,15,15	1.34	2 (14%)	15,20,20	1.35	3 (20%)

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
3	GOL	B	504	-	-	1/4/4/4	-
3	GOL	C	503	-	-	3/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	D	502	-	-	1/4/4/4	-
2	HEM	A	501	1	-	3/14/54/54	-
3	GOL	A	505	-	-	4/4/4/4	-
3	GOL	C	506	-	-	4/4/4/4	-
4	KYN	B	503	-	-	4/12/12/12	0/1/1/1
3	GOL	A	504	-	-	4/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
4	KYN	B	505	-	-	8/12/12/12	0/1/1/1
2	HEM	B	501	5,1	-	4/14/54/54	-
2	HEM	C	501	1	-	3/14/54/54	-
3	GOL	D	504	-	-	2/4/4/4	-
4	KYN	B	502[A]	-	-	9/12/12/12	0/1/1/1
2	HEM	D	501	1	-	4/14/54/54	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
4	KYN	B	502[B]	-	-	9/12/12/12	0/1/1/1
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
4	KYN	A	506	-	-	5/12/12/12	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NB	7.44	2.17	1.94
2	A	501	HEM	FE-NB	6.39	2.14	1.94
2	D	501	HEM	FE-NA	5.67	2.13	1.95
2	B	501	HEM	FE-NA	5.53	2.13	1.95
2	A	501	HEM	FE-NA	5.41	2.13	1.95
2	D	501	HEM	FE-NB	5.29	2.11	1.94
2	C	501	HEM	FE-NC	5.16	2.12	1.95
2	C	501	HEM	FE-NA	4.35	2.09	1.95
2	C	501	HEM	FE-NB	4.22	2.07	1.94
2	D	501	HEM	FE-NC	3.85	2.07	1.95
4	B	505	KYN	CD2-C1	3.09	1.54	1.48
4	B	503	KYN	CD2-C1	2.92	1.54	1.48
2	A	501	HEM	FE-NC	2.89	2.04	1.95
4	B	502[A]	KYN	CD2-C1	2.85	1.54	1.48
2	A	501	HEM	CAB-C3B	2.80	1.54	1.47
2	A	501	HEM	CAC-C3C	2.79	1.54	1.47
4	B	502[B]	KYN	CD2-C1	2.78	1.53	1.48
2	B	501	HEM	CAB-C3B	2.74	1.54	1.47
2	D	501	HEM	CMC-C2C	2.69	1.56	1.50
4	B	505	KYN	CG-N1	2.65	1.46	1.38
4	B	503	KYN	CB-C1	2.58	1.54	1.51
4	B	503	KYN	CG-N1	2.56	1.46	1.38
4	A	506	KYN	CG-N1	2.54	1.46	1.38
2	B	501	HEM	CAC-C3C	2.45	1.53	1.47
3	D	502	GOL	C1-C2	2.41	1.60	1.51
2	C	501	HEM	CMC-C2C	2.38	1.55	1.50
4	B	502[B]	KYN	CG-N1	2.37	1.45	1.38
2	A	501	HEM	CMC-C2C	2.36	1.55	1.50
2	C	501	HEM	CMB-C2B	2.32	1.55	1.50
4	B	502[A]	KYN	CB-C1	2.30	1.54	1.51
4	B	502[B]	KYN	CB-C1	2.30	1.54	1.51
2	B	501	HEM	CMB-C2B	2.29	1.55	1.50
2	D	501	HEM	CMB-C2B	2.27	1.55	1.50
2	D	501	HEM	CAC-C3C	2.26	1.53	1.47
4	B	502[A]	KYN	CG-N1	2.23	1.45	1.38
2	C	501	HEM	CAC-C3C	2.21	1.53	1.47
4	B	503	KYN	CD2-CG	-2.21	1.38	1.41
2	D	501	HEM	CAB-C3B	2.20	1.53	1.47
2	B	501	HEM	CMC-C2C	2.19	1.55	1.50
2	C	501	HEM	CAB-C3B	2.17	1.53	1.47
3	A	504	GOL	C1-C2	2.14	1.60	1.51
4	B	505	KYN	O2-C1	-2.13	1.18	1.22
4	A	506	KYN	CD2-C1	2.08	1.52	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CMD-C2D	2.08	1.55	1.50
2	A	501	HEM	CMB-C2B	2.07	1.55	1.50
2	D	501	HEM	C3B-C2B	-2.01	1.33	1.37

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C4B-NB	-4.90	105.95	109.47
2	C	501	HEM	C3B-C4B-NB	-4.41	106.30	109.47
4	B	505	KYN	CB-C1-CD2	4.39	124.94	119.82
4	B	505	KYN	O2-C1-CB	-3.98	115.97	120.70
2	A	501	HEM	C4D-ND-C1D	3.75	109.65	105.21
2	B	501	HEM	C4D-ND-C1D	3.73	109.62	105.21
2	D	501	HEM	C4C-C3C-C2C	3.44	109.80	106.81
2	C	501	HEM	C4C-C3C-C2C	3.39	109.76	106.81
2	B	501	HEM	C3D-C4D-ND	-3.38	106.46	110.17
2	A	501	HEM	CHA-C4D-ND	3.28	128.43	124.37
2	D	501	HEM	C4D-ND-C1D	3.26	109.07	105.21
2	A	501	HEM	CAD-CBD-CGD	-3.23	105.11	113.67
2	B	501	HEM	C4C-C3C-C2C	3.21	109.60	106.81
2	C	501	HEM	CMC-C2C-C1C	3.19	130.35	124.73
2	D	501	HEM	C4B-C3B-C2B	3.07	110.10	107.28
2	D	501	HEM	C3D-C4D-ND	-3.05	106.82	110.17
2	D	501	HEM	C1B-NB-C4B	3.01	108.78	105.21
2	A	501	HEM	C2D-C1D-ND	-2.96	106.48	109.90
2	A	501	HEM	C3D-C4D-ND	-2.95	106.94	110.17
2	C	501	HEM	CAD-CBD-CGD	-2.83	106.17	113.67
2	B	501	HEM	C3B-C4B-NB	-2.80	107.46	109.47
2	C	501	HEM	C1B-NB-C4B	2.77	108.48	105.21
4	B	503	KYN	CD2-CG-N1	-2.70	118.92	122.68
4	A	506	KYN	OXT-C-O	-2.67	118.02	124.08
2	C	501	HEM	C4D-ND-C1D	2.66	108.36	105.21
2	C	501	HEM	C4B-C3B-C2B	2.65	109.71	107.28
2	C	501	HEM	CMC-C2C-C3C	-2.62	122.08	128.43
2	D	501	HEM	C2D-C1D-ND	-2.60	106.90	109.90
2	D	501	HEM	CHD-C1D-ND	2.49	127.11	124.42
2	A	501	HEM	CHD-C4C-C3C	2.46	129.36	125.21
2	D	501	HEM	C2A-C1A-NA	-2.46	107.43	110.15
2	B	501	HEM	C1B-NB-C4B	2.44	108.10	105.21
2	B	501	HEM	C2D-C1D-ND	-2.42	107.10	109.90
2	D	501	HEM	CMC-C2C-C1C	2.40	128.96	124.73
2	D	501	HEM	C4C-NC-C1C	2.39	109.72	105.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1B-NB-C4B	2.37	108.01	105.21
2	A	501	HEM	C3B-C4B-NB	-2.34	107.78	109.47
2	A	501	HEM	C4C-C3C-C2C	2.34	108.84	106.81
2	C	501	HEM	CHA-C4D-ND	2.29	127.20	124.37
4	B	502[A]	KYN	CA-CB-C1	-2.28	110.62	113.06
4	B	502[B]	KYN	CA-CB-C1	-2.28	110.62	113.06
2	C	501	HEM	CHD-C1D-ND	2.27	126.87	124.42
2	D	501	HEM	CMB-C2B-C1B	2.26	128.56	125.03
2	B	501	HEM	CHD-C4C-C3C	2.25	129.00	125.21
2	A	501	HEM	CHC-C1C-NC	2.25	126.90	124.45
2	A	501	HEM	CHD-C1D-ND	2.24	126.83	124.42
2	B	501	HEM	CHA-C4D-ND	2.23	127.12	124.37
2	B	501	HEM	C2A-C1A-NA	-2.23	107.68	110.15
2	C	501	HEM	C2D-C1D-ND	-2.22	107.34	109.90
3	C	506	GOL	O3-C3-C2	-2.22	100.39	110.38
2	D	501	HEM	C1D-C2D-C3D	2.20	109.29	106.98
2	B	501	HEM	CAC-C3C-C2C	-2.20	121.29	128.43
2	C	501	HEM	C3D-C4D-ND	-2.17	107.79	110.17
2	C	501	HEM	CAC-C3C-C2C	-2.17	121.38	128.43
4	B	503	KYN	OXT-C-O	-2.14	119.23	124.08
2	B	501	HEM	CAA-CBA-CGA	-2.13	108.02	113.67
4	A	506	KYN	O2-C1-CD2	-2.12	117.32	120.79
2	C	501	HEM	C4C-NC-C1C	2.10	109.24	105.82
2	C	501	HEM	CMB-C2B-C1B	2.09	128.30	125.03
4	A	506	KYN	CE2-CD2-CG	2.09	121.07	118.96
2	B	501	HEM	CHC-C1C-NC	2.08	126.72	124.45
2	C	501	HEM	CHD-C4C-C3C	2.07	128.70	125.21
3	D	505	GOL	C3-C2-C1	-2.06	104.24	111.80
2	B	501	HEM	CMC-C2C-C1C	2.05	128.34	124.73
2	A	501	HEM	C4C-NC-C1C	2.04	109.14	105.82
2	A	501	HEM	CAC-C3C-C2C	-2.03	121.82	128.43
2	B	501	HEM	C4C-NC-C1C	2.02	109.11	105.82
2	D	501	HEM	O2A-CGA-CBA	2.01	120.36	114.00
2	D	501	HEM	CHC-C4B-NB	2.01	126.59	124.42
2	B	501	HEM	C4B-C3B-C2B	2.00	109.12	107.28
4	B	505	KYN	OXT-C-O	-2.00	119.54	124.08

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3
3	A	504	GOL	C1-C2-C3-O3
3	A	505	GOL	O1-C1-C2-C3
3	A	507	GOL	O1-C1-C2-O2
3	A	507	GOL	O1-C1-C2-C3
3	B	507	GOL	O1-C1-C2-C3
3	C	502	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-C3
3	C	505	GOL	O1-C1-C2-C3
3	C	506	GOL	O1-C1-C2-C3
3	C	506	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	D	505	GOL	C1-C2-C3-O3
4	A	506	KYN	C-CA-CB-C1
4	B	503	KYN	O-C-CA-N
4	B	505	KYN	CB-C1-CD2-CG
4	B	505	KYN	C-CA-CB-C1
4	B	505	KYN	N-CA-CB-C1
3	D	503	GOL	O1-C1-C2-O2
4	B	502[A]	KYN	O2-C1-CB-CA
4	B	502[B]	KYN	O2-C1-CB-CA
4	B	502[A]	KYN	CD2-C1-CB-CA
4	B	502[B]	KYN	CD2-C1-CB-CA
4	B	503	KYN	OXT-C-CA-N
3	A	505	GOL	C1-C2-C3-O3
3	B	504	GOL	O1-C1-C2-C3
3	D	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O2-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	B	507	GOL	O1-C1-C2-O2
3	C	502	GOL	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-O2
3	C	506	GOL	O1-C1-C2-O2
4	B	505	KYN	O2-C1-CB-CA
4	B	505	KYN	CD2-C1-CB-CA
4	B	502[A]	KYN	CB-C1-CD2-CE2
4	B	502[A]	KYN	O2-C1-CD2-CE2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	502[B]	KYN	O2-C1-CD2-CG
4	B	505	KYN	O2-C1-CD2-CG
4	A	506	KYN	N-CA-CB-C1
4	B	502[A]	KYN	N-CA-CB-C1
4	B	502[B]	KYN	N-CA-CB-C1
3	A	504	GOL	O1-C1-C2-O2
3	A	504	GOL	O2-C2-C3-O3
3	C	506	GOL	O2-C2-C3-O3
3	D	505	GOL	O2-C2-C3-O3
4	B	502[B]	KYN	O2-C1-CD2-CE2
3	C	505	GOL	O1-C1-C2-O2
4	B	502[A]	KYN	C-CA-CB-C1
4	B	502[B]	KYN	C-CA-CB-C1
3	D	504	GOL	O1-C1-C2-O2
3	D	504	GOL	O2-C2-C3-O3
4	A	506	KYN	OXT-C-CA-CB
4	A	506	KYN	O-C-CA-CB
4	B	503	KYN	O-C-CA-CB
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4C-C3C-CAC-CBC
2	C	501	HEM	C4B-C3B-CAB-CBB
4	B	503	KYN	OXT-C-CA-CB
4	B	502[B]	KYN	CB-C1-CD2-CE2
4	B	502[A]	KYN	O2-C1-CD2-CG
2	B	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O2D
3	C	503	GOL	O2-C2-C3-O3
4	B	505	KYN	OXT-C-CA-N
2	D	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4C-C3C-CAC-CBC
4	B	502[A]	KYN	CB-C1-CD2-CG
4	B	502[B]	KYN	CB-C1-CD2-CG
4	A	506	KYN	OXT-C-CA-N
4	B	502[A]	KYN	O-C-CA-CB
4	B	502[B]	KYN	O-C-CA-CB

Continued on next page...

Continued from previous page...

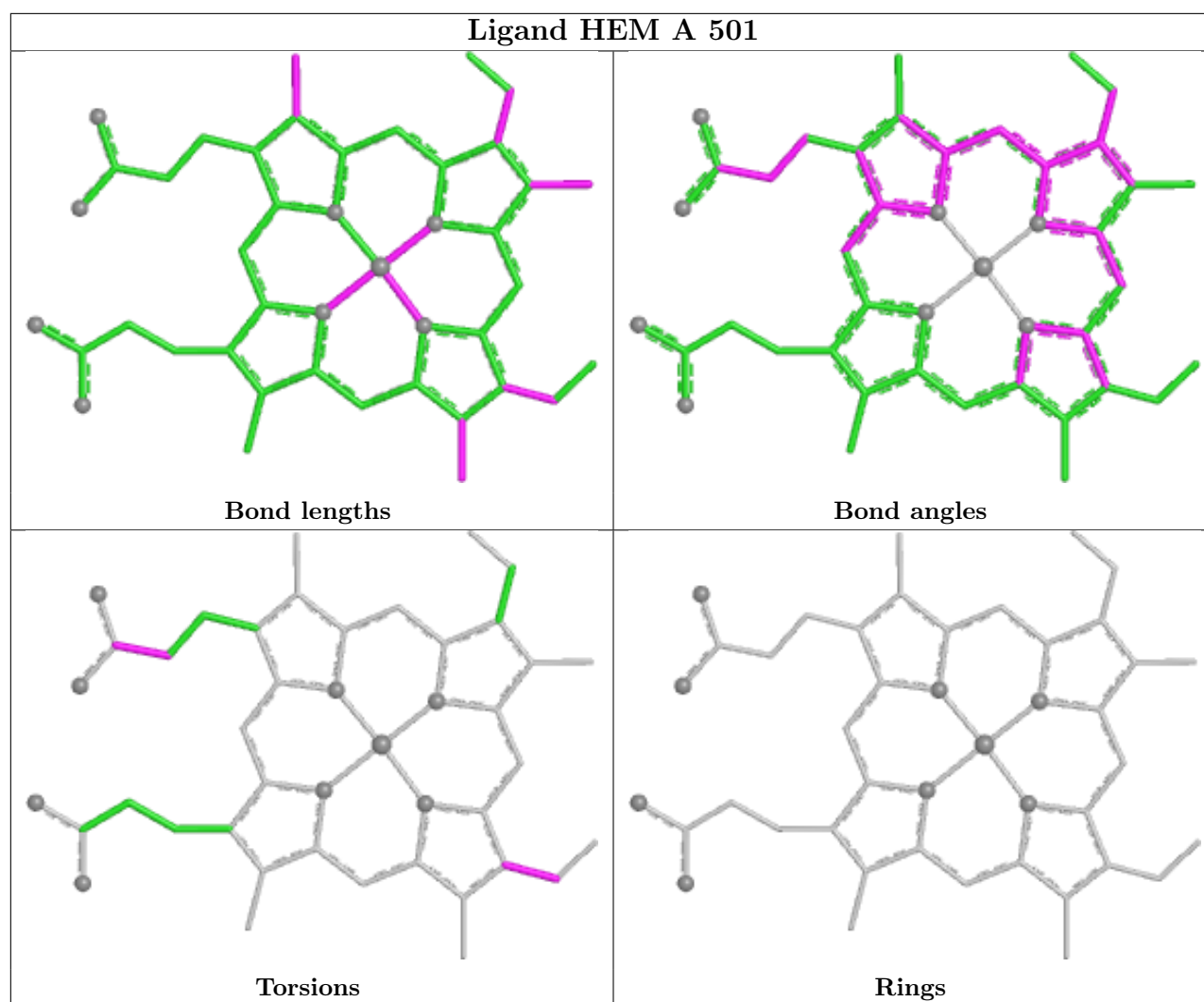
Mol	Chain	Res	Type	Atoms
4	B	505	KYN	O-C-CA-N

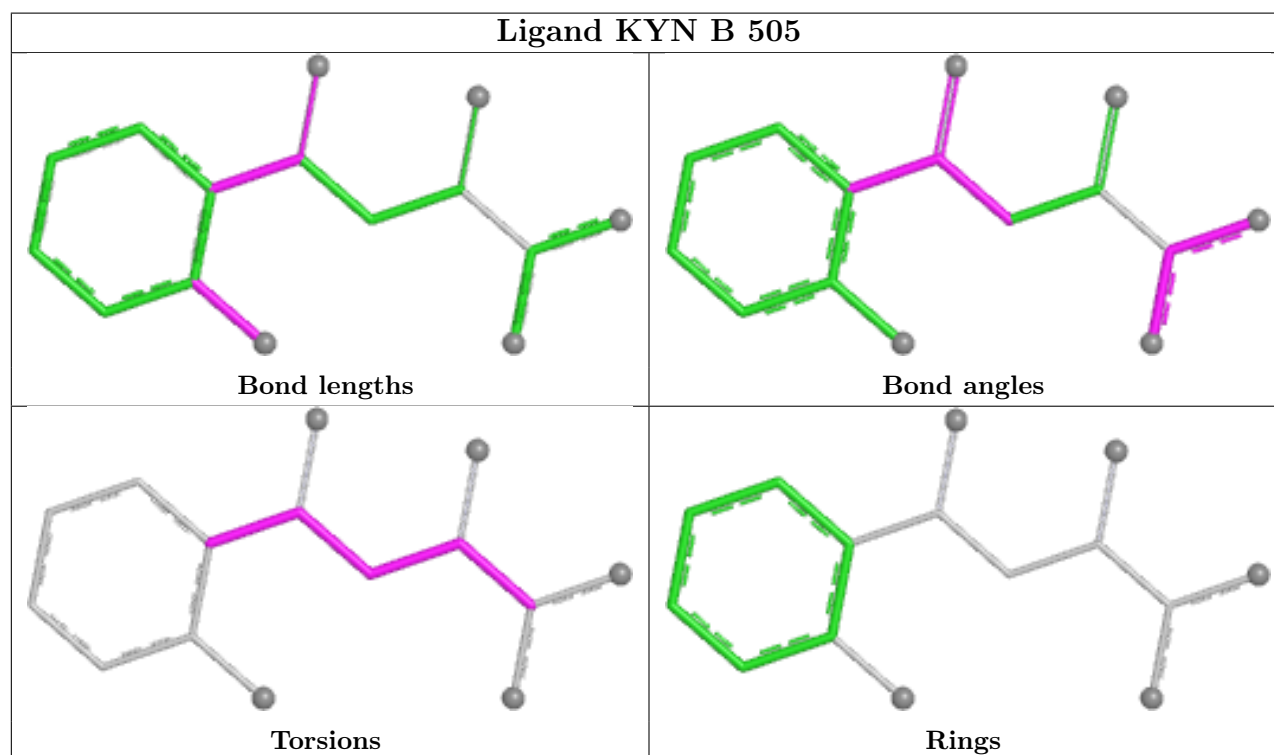
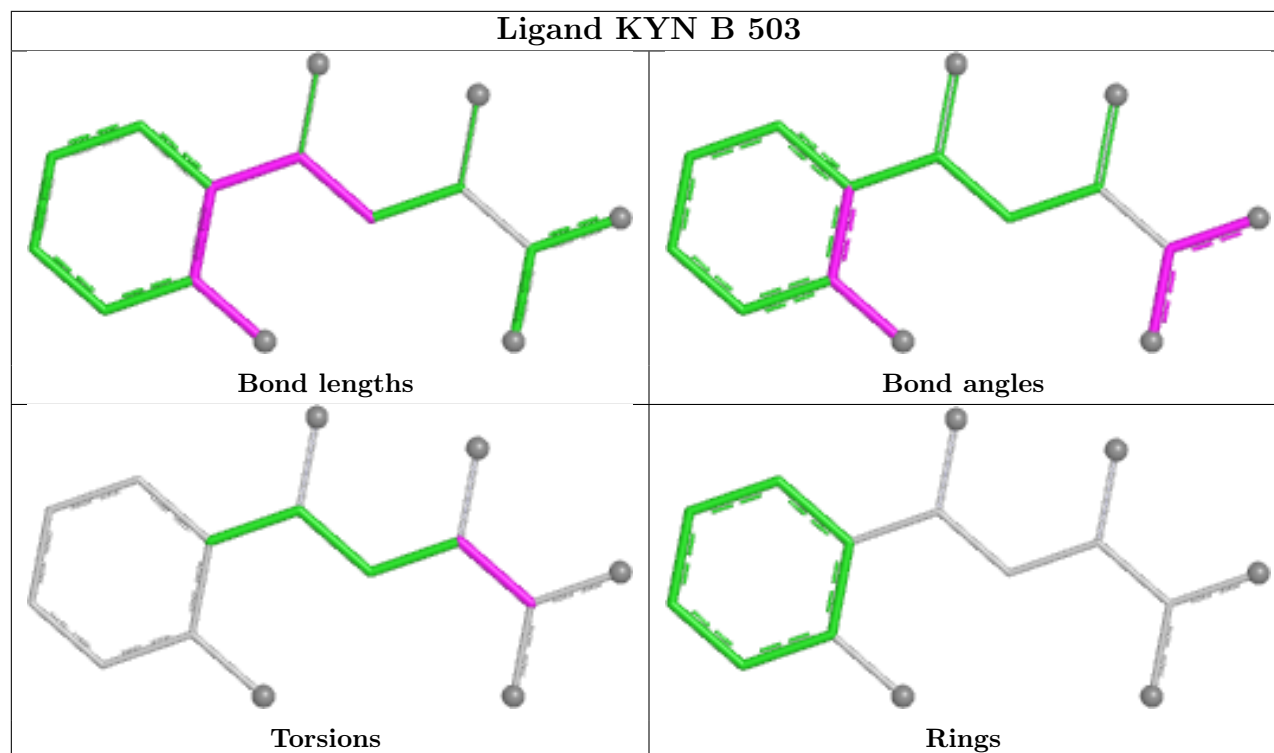
There are no ring outliers.

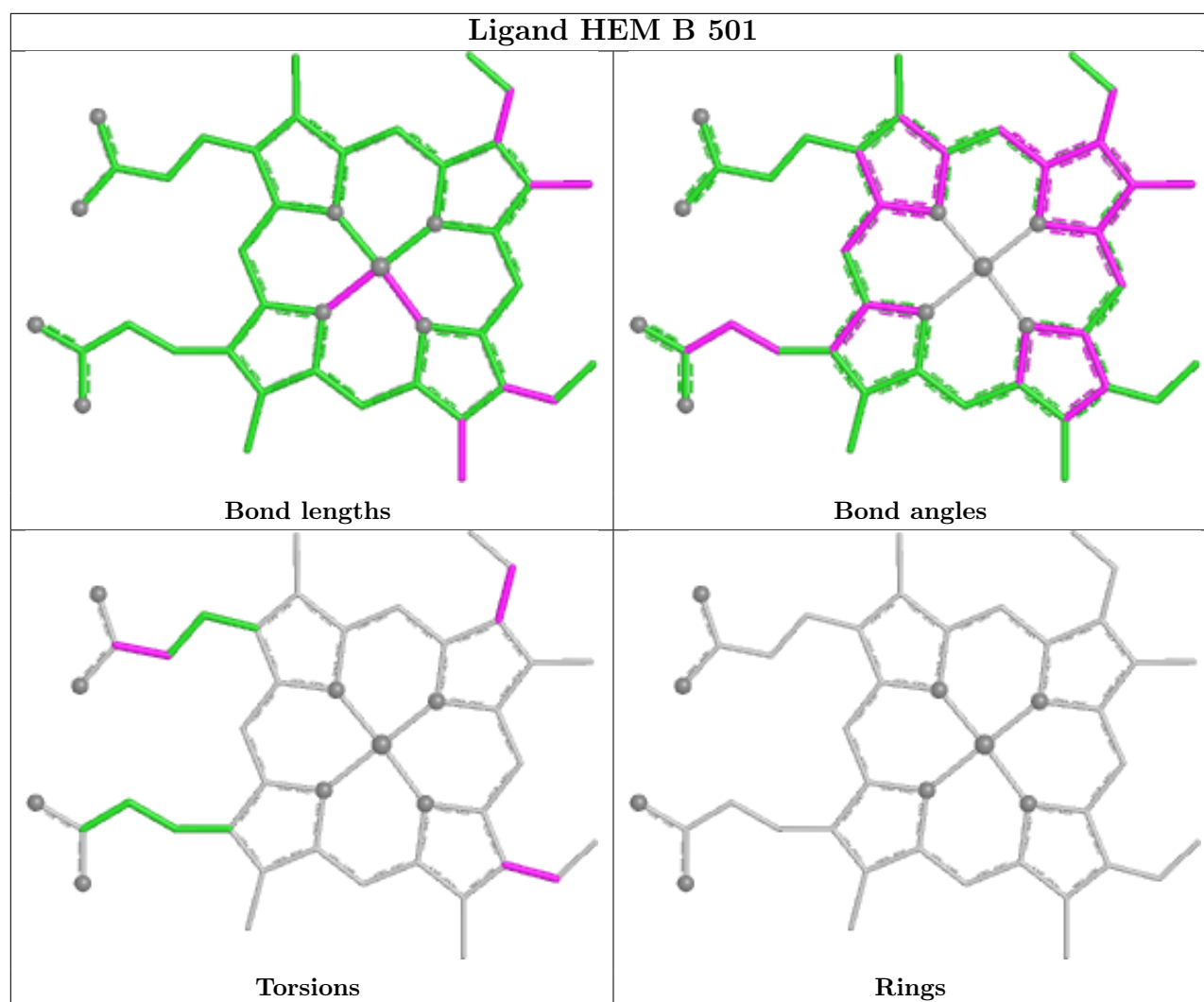
15 monomers are involved in 47 short contacts:

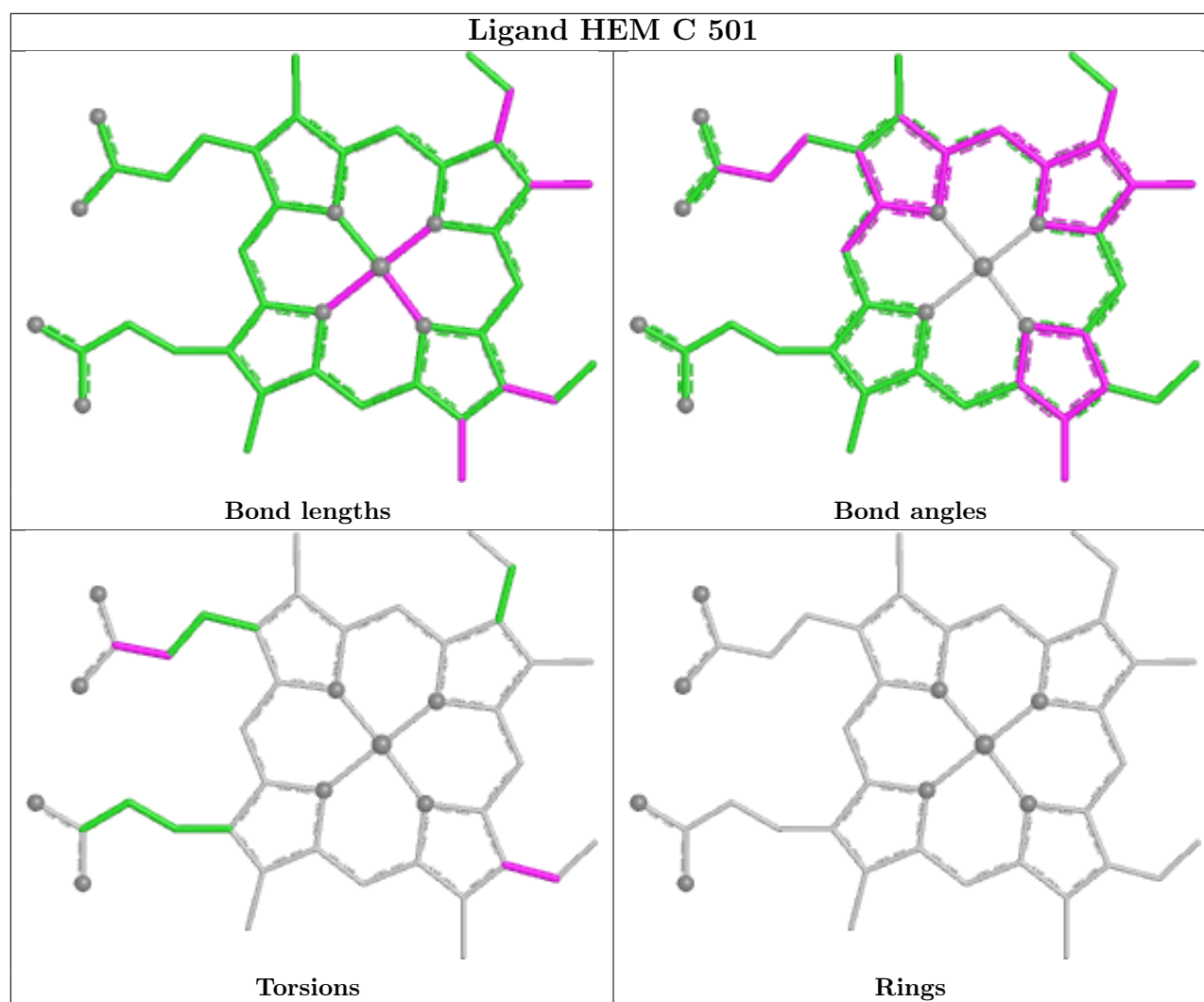
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	GOL	1	0
3	C	502	GOL	2	0
2	A	501	HEM	7	0
5	B	506[B]	OXY	1	0
3	C	506	GOL	2	0
4	B	503	KYN	3	0
3	A	504	GOL	1	0
4	B	505	KYN	4	0
2	B	501	HEM	7	0
2	C	501	HEM	4	0
2	D	501	HEM	7	0
3	A	503	GOL	1	0
3	C	505	GOL	3	0
4	B	502[B]	KYN	1	0
4	A	506	KYN	3	0

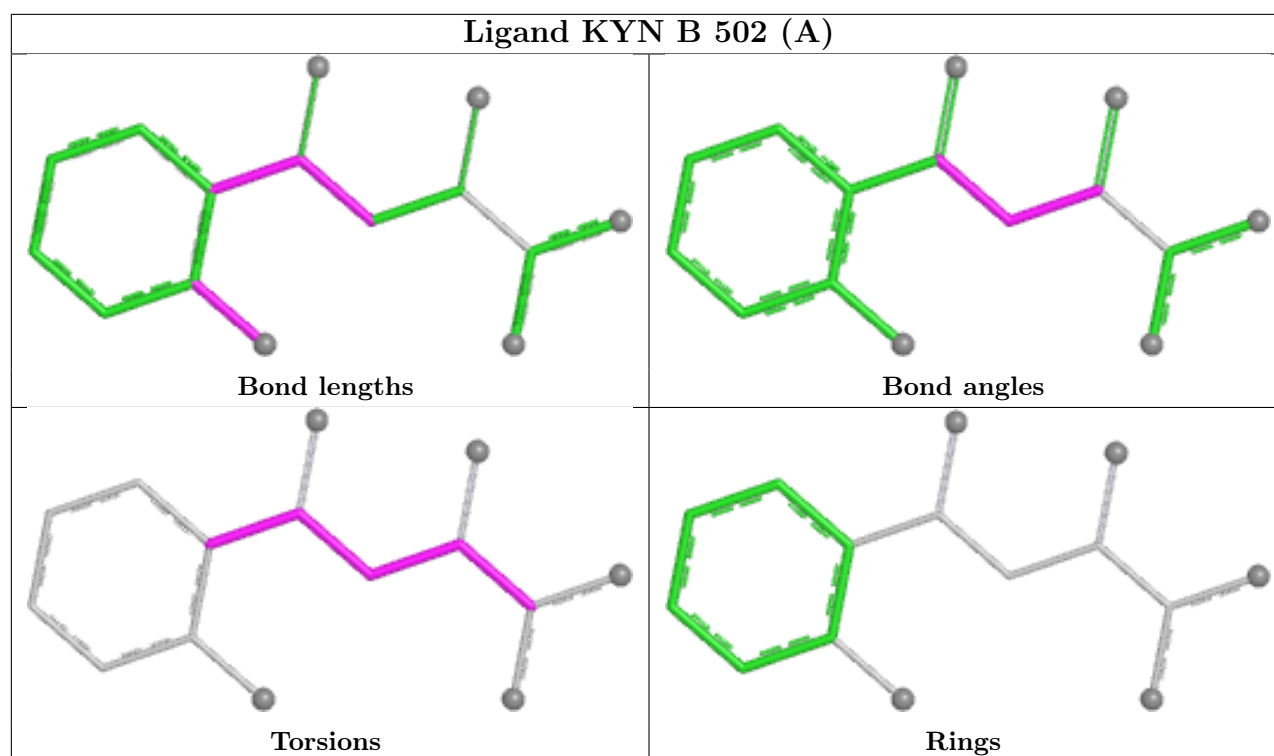
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

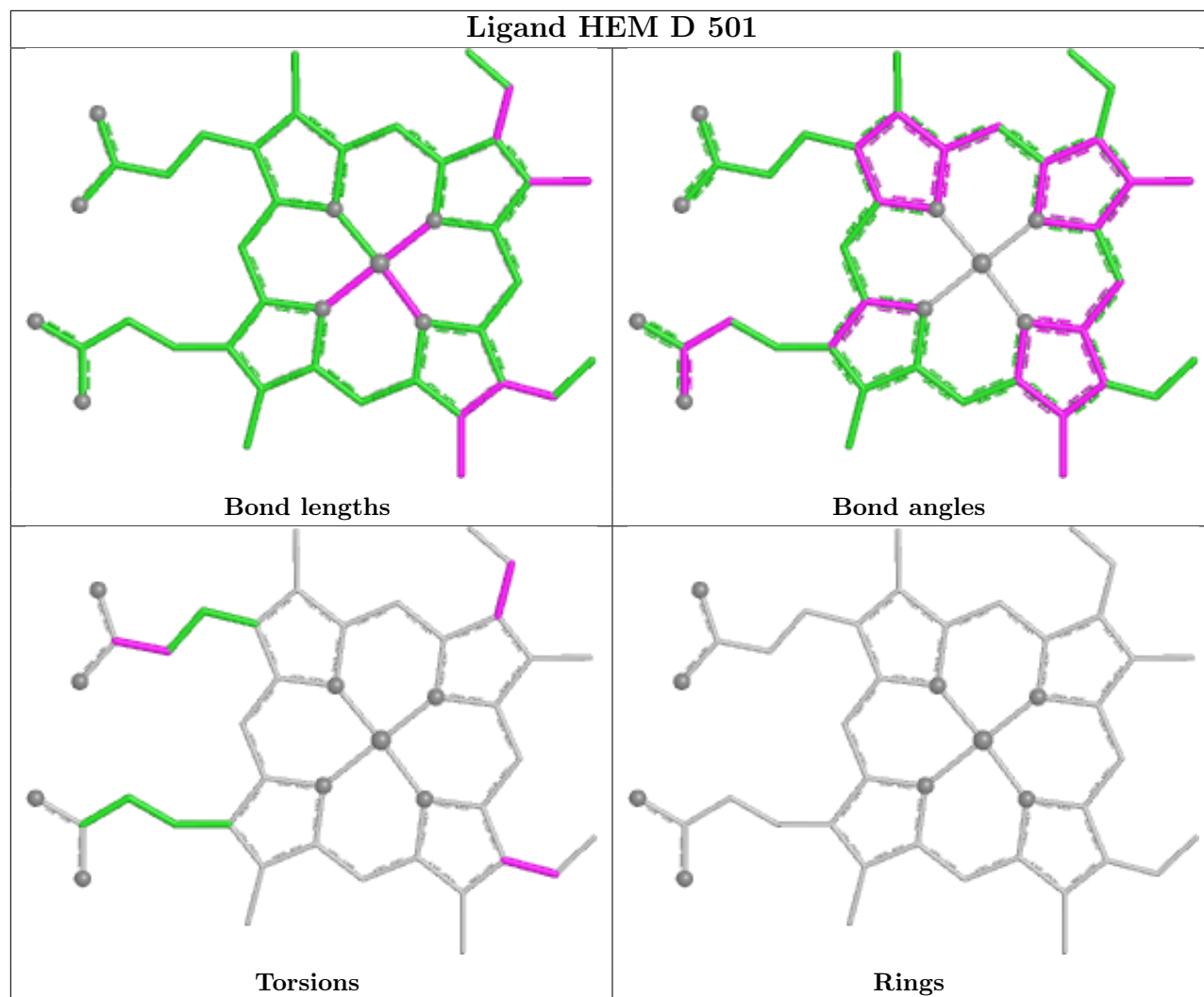


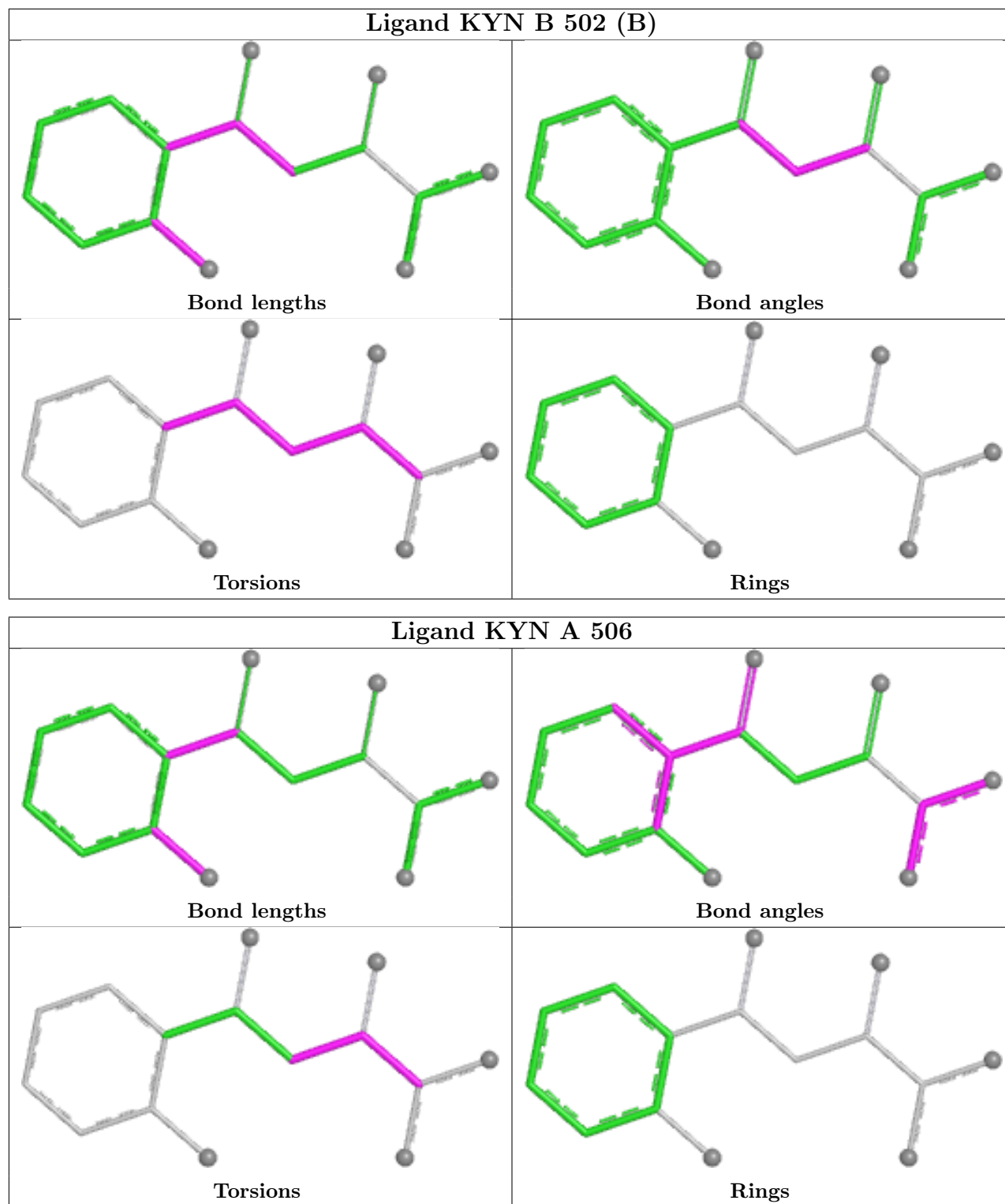












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.22	9 (2%) 59 61	23, 42, 72, 99	1 (0%)
1	B	381/405 (94%)	-0.06	20 (5%) 33 33	24, 46, 80, 107	7 (1%)
1	C	372/405 (91%)	-0.18	8 (2%) 62 63	28, 44, 67, 92	1 (0%)
1	D	373/405 (92%)	-0.26	9 (2%) 59 61	27, 42, 66, 101	1 (0%)
All	All	1496/1620 (92%)	-0.18	46 (3%) 51 52	23, 43, 72, 107	10 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	THR	5.2
1	B	376	ALA	5.0
1	B	379	THR	4.8
1	C	362	PRO	4.6
1	B	380	GLY	4.4
1	B	11	GLY	4.2
1	B	282	THR	4.1
1	B	13	ALA	4.0
1	A	285	GLY	4.0
1	D	403	GLY	3.7
1	C	381	GLY	3.6
1	B	362	PRO	3.5
1	B	12	SER	3.4
1	B	374	LEU	3.3
1	B	284	GLY	3.2
1	C	262	GLY	3.2
1	A	283	ALA	3.1
1	D	14	ALA	3.1
1	D	362	PRO	3.0
1	A	14	ALA	2.9
1	A	284	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	13	ALA	2.8
1	B	189	GLN	2.7
1	B	283	ALA	2.7
1	D	382	THR	2.6
1	B	287	HIS	2.5
1	D	381	GLY	2.5
1	C	283	ALA	2.5
1	D	262	GLY	2.4
1	B	291	PHE	2.4
1	C	284	GLY	2.3
1	C	361	GLN	2.3
1	B	377	LYS	2.3
1	B	262	GLY	2.3
1	A	263	SER	2.3
1	A	190	MET	2.3
1	A	381	GLY	2.2
1	C	287	HIS	2.1
1	B	375	GLU	2.1
1	B	401	LYS	2.1
1	C	285	GLY	2.1
1	A	382	THR	2.1
1	B	402	GLU	2.1
1	B	285	GLY	2.0
1	D	287	HIS	2.0
1	D	265	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

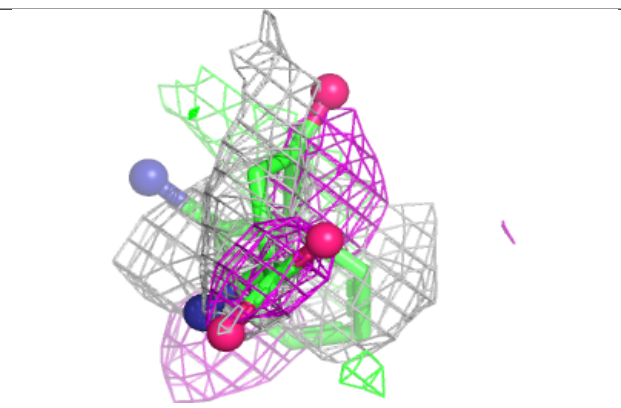
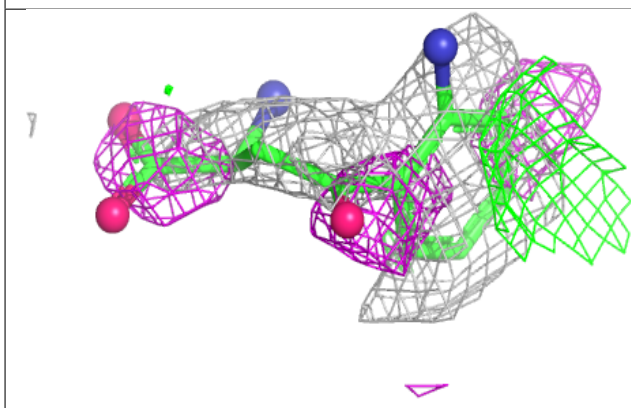
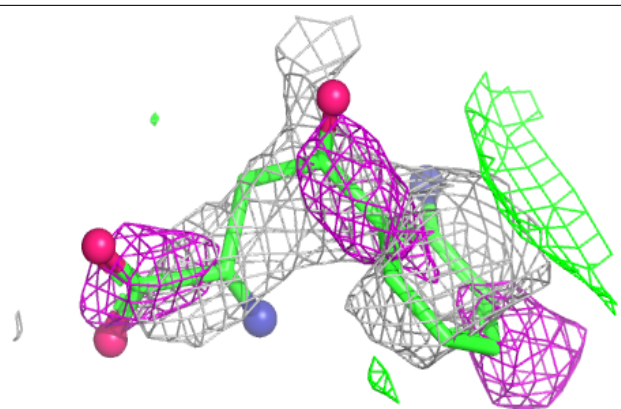
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OXY	C	504	2/2	0.74	0.14	67,67,67,68	0
3	GOL	B	507	6/6	0.75	0.19	80,84,92,94	0
3	GOL	C	505	6/6	0.78	0.19	59,66,69,69	0
4	KYN	B	502[A]	15/15	0.78	0.20	59,67,83,87	7
4	KYN	B	502[B]	15/15	0.78	0.20	59,68,83,87	7
3	GOL	A	507	6/6	0.78	0.16	73,79,79,82	0
4	KYN	A	506	15/15	0.79	0.22	40,46,53,54	15
4	KYN	B	503	15/15	0.80	0.18	42,52,59,63	15
3	GOL	C	503	6/6	0.81	0.20	57,59,66,69	0
3	GOL	A	505	6/6	0.82	0.23	50,59,65,66	0
3	GOL	B	504	6/6	0.83	0.23	51,57,61,67	0
3	GOL	D	504	6/6	0.84	0.18	61,64,67,69	0
3	GOL	C	502	6/6	0.85	0.12	49,53,58,60	0
3	GOL	D	503	6/6	0.85	0.17	56,58,66,70	0
4	KYN	B	505	15/15	0.86	0.17	40,48,54,56	15
3	GOL	C	506	6/6	0.87	0.15	42,46,48,54	0
5	OXY	B	506[B]	2/2	0.88	0.15	54,54,54,55	2
3	GOL	D	502	6/6	0.88	0.13	42,51,54,58	0
3	GOL	A	502	6/6	0.89	0.16	48,53,54,56	0
3	GOL	A	504	6/6	0.91	0.17	53,63,66,71	0
3	GOL	A	503	6/6	0.92	0.12	46,52,54,55	0
2	HEM	D	501	43/43	0.94	0.10	34,43,58,65	0
2	HEM	B	501	43/43	0.94	0.11	35,52,66,69	0
2	HEM	A	501	43/43	0.95	0.10	37,51,66,67	0
2	HEM	C	501	43/43	0.95	0.09	37,45,57,64	0
3	GOL	D	505	6/6	0.96	0.09	40,42,43,45	0

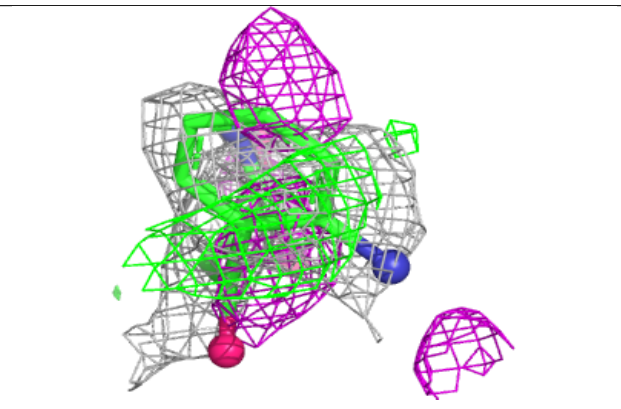
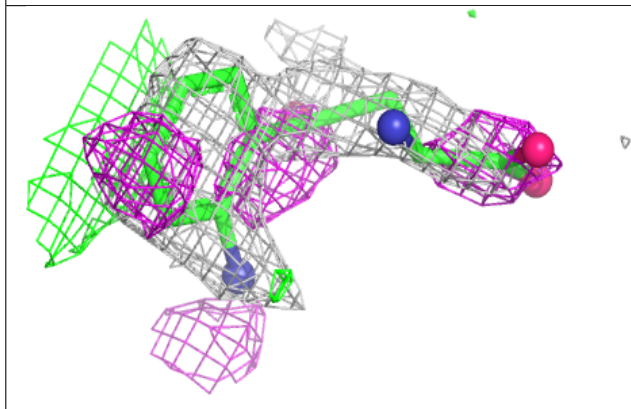
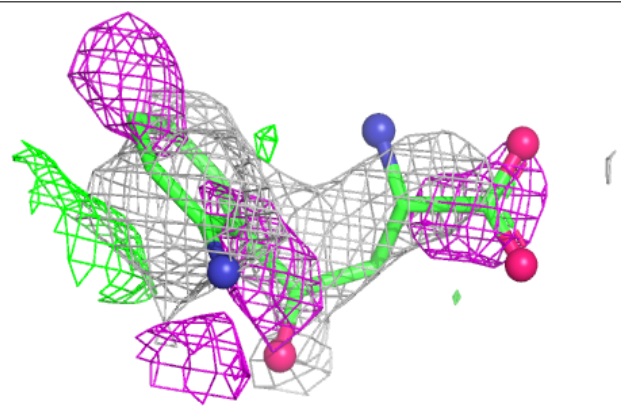
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KYN B 502 (A):

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

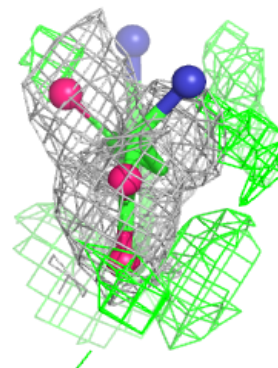
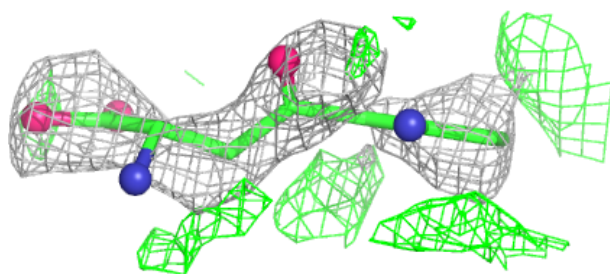
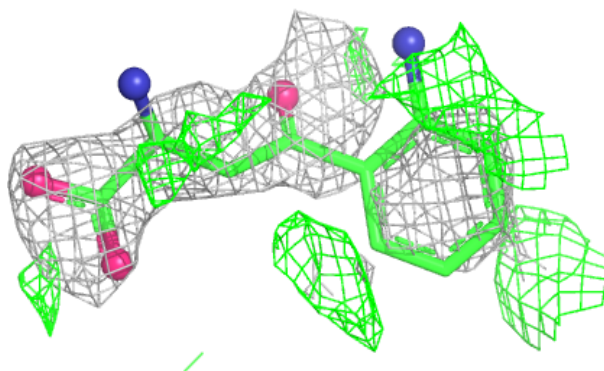
**Electron density around KYN B 502 (B):**

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

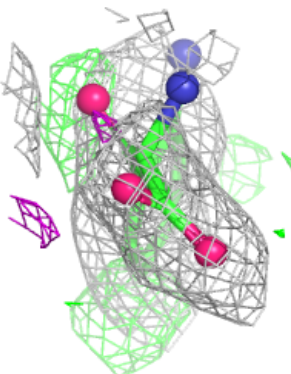
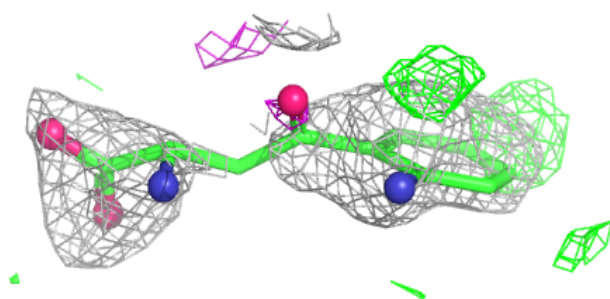
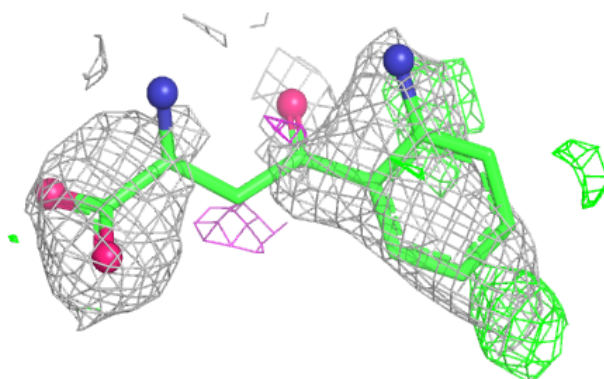


Electron density around KYN A 506:

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

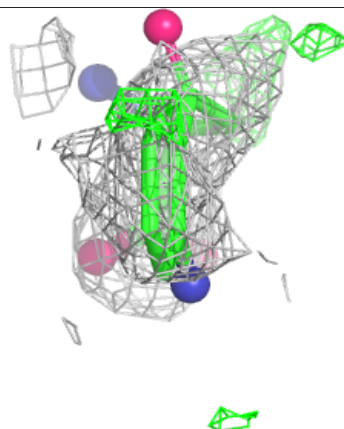
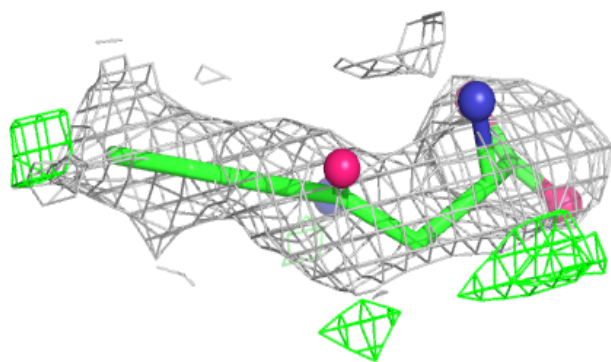
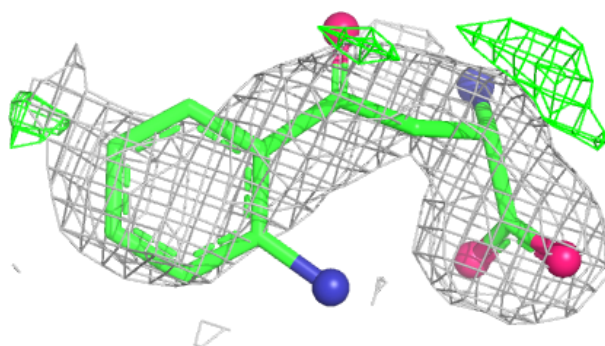
**Electron density around KYN B 503:**

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



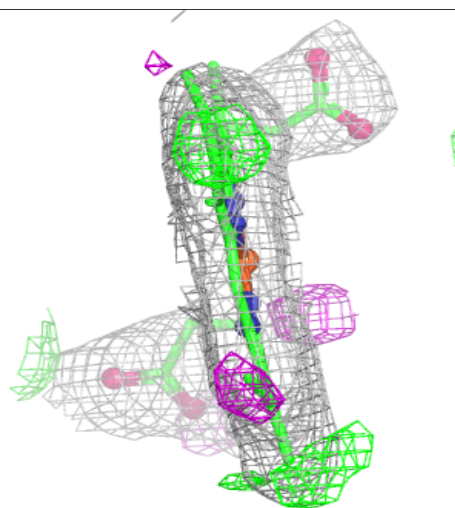
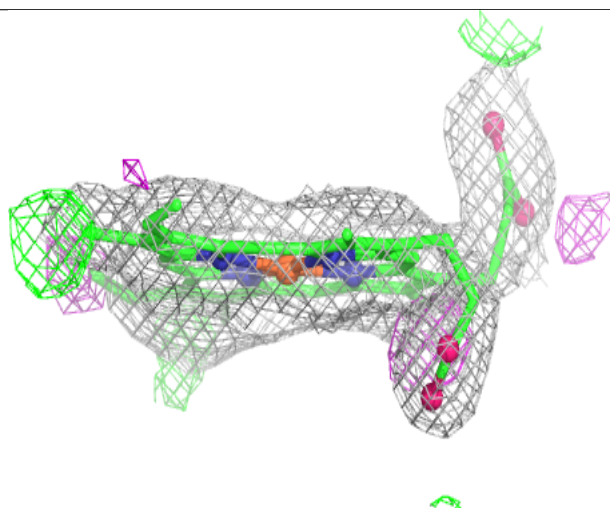
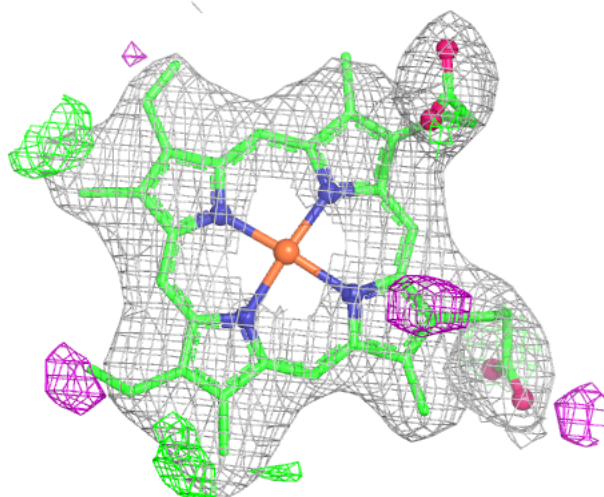
Electron density around KYN B 505:

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



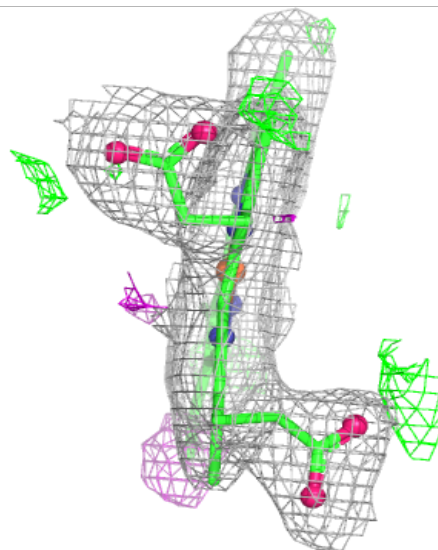
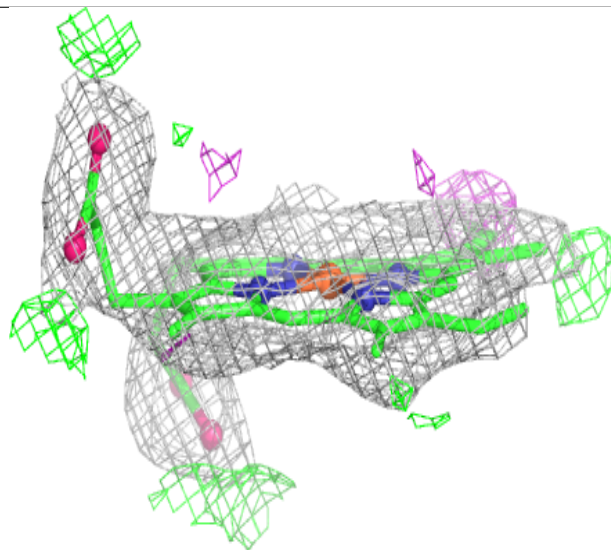
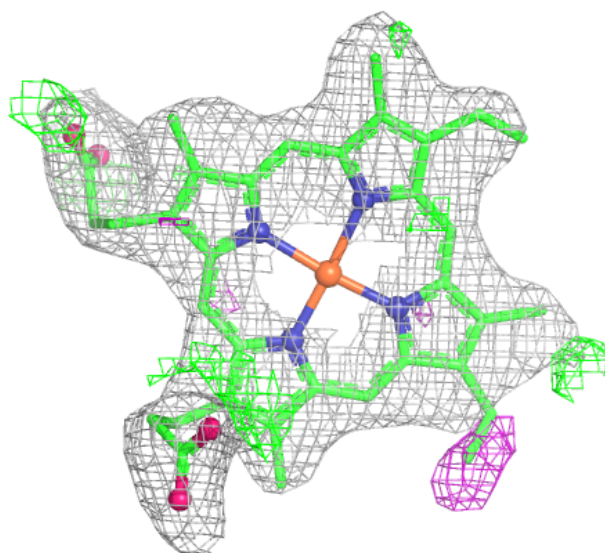
Electron density around HEM D 501:

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



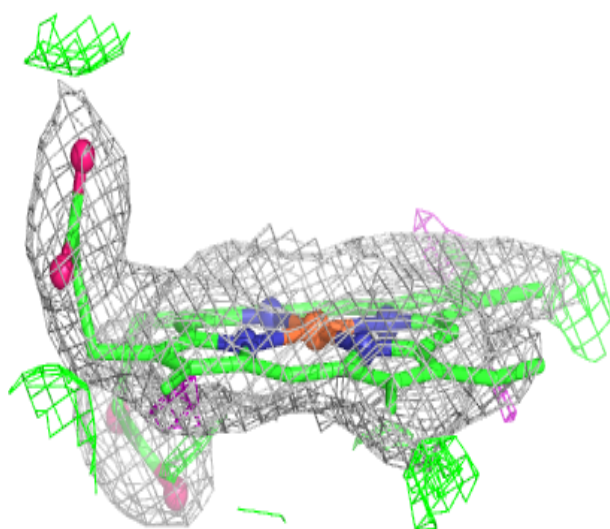
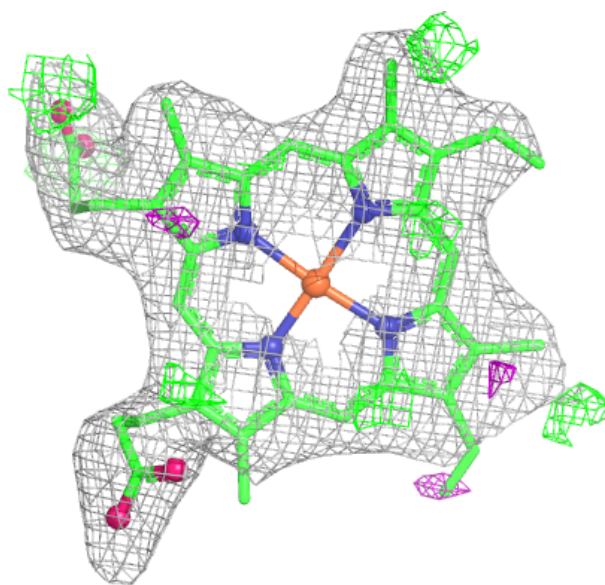
Electron density around HEM B 501:

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



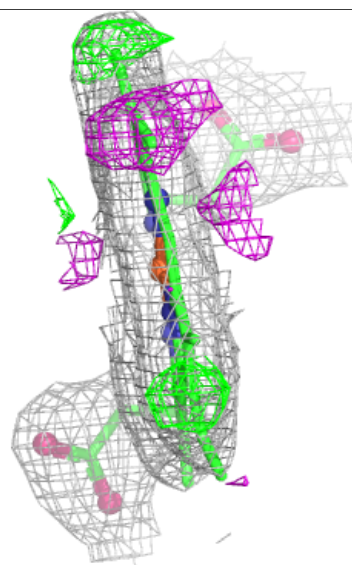
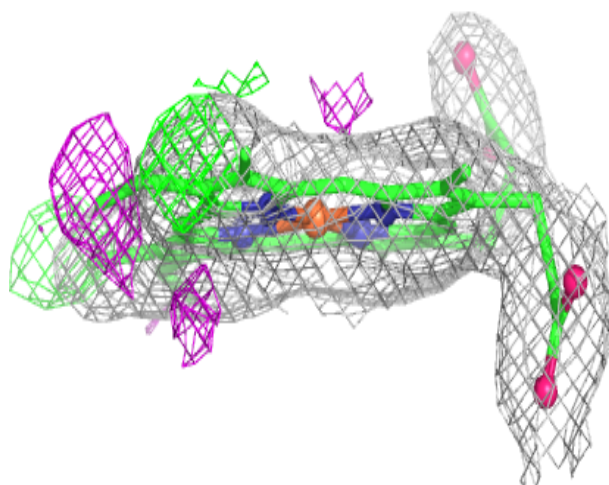
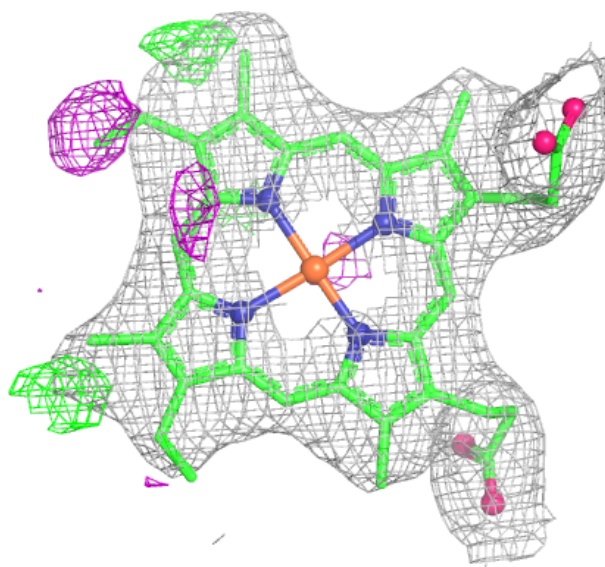
Electron density around HEM A 501:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.