



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:33 AM UTC

PDB ID : 7ABN / pdb_00007abn
Title : Structure of the reversible pyrrole-2-carboxylic acid decarboxylase
PA0254/HudA
Authors : Leys, D.
Deposited on : 2020-09-08
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

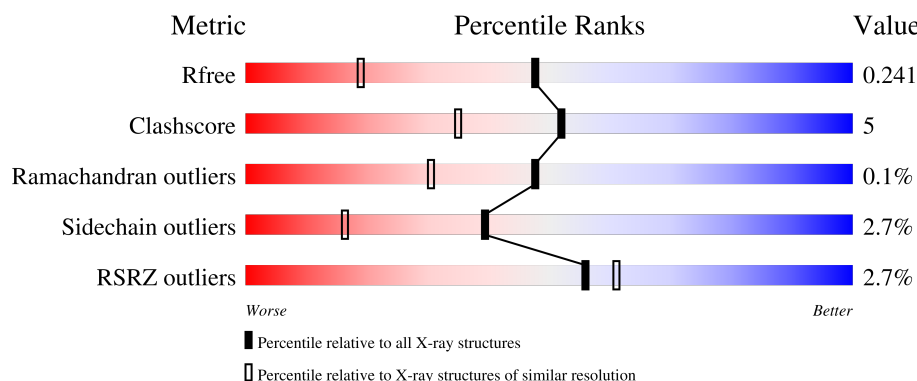
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	496	
1	D	496	
1	H	496	
1	M	496	

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
5	IMD	A	504	-	-	X	-
5	IMD	D	504	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16967 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 UbiD-like decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	496	Total	C	N	O	S	0	1	0
			3841	2439	697	690	15			
1	A	496	Total	C	N	O	S	0	0	0
			3848	2441	702	690	15			
1	H	494	Total	C	N	O	S	0	0	0
			3830	2432	697	686	15			
1	M	494	Total	C	N	O	S	0	2	0
			3852	2445	702	690	15			

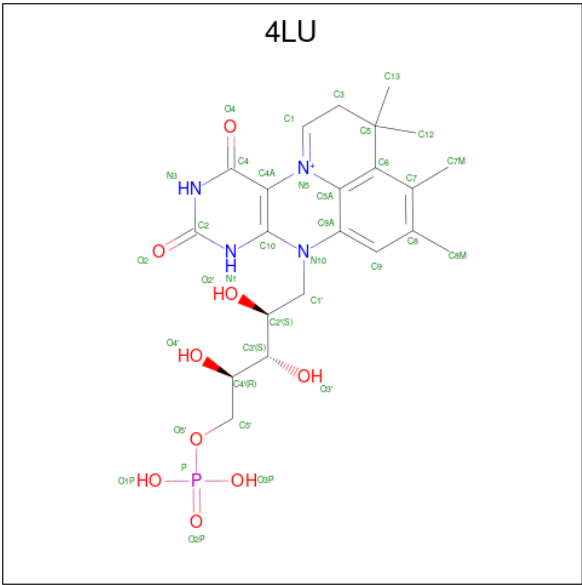
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	M	1	Total	Mn	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

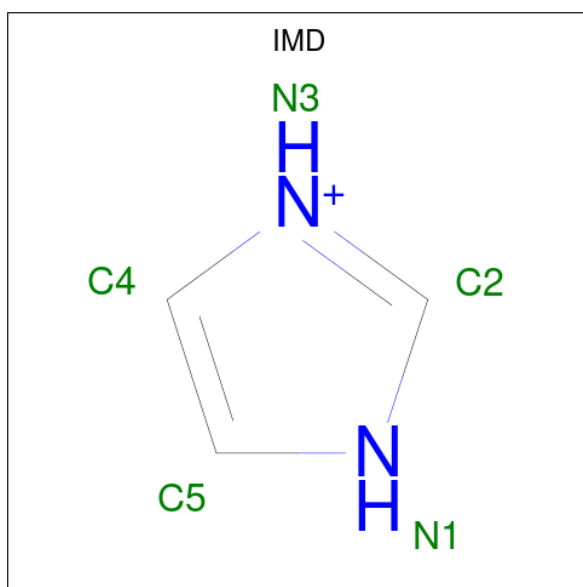
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

- Molecule 4 is 1-deoxy-5-O-phosphono-1-(3,3,4,5-tetramethyl-9,11-dioxo-2,3,8,9,10,11-hexahydro-7H-quinolino[1,8-fg]pteridin-12-ium-7-yl)-D-ribose (CCD ID: 4LU) (formula: C₂₂H₃₀N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			36	22	4	9	1		
4	A	1	Total	C	N	O	P	0	0
			36	22	4	9	1		
4	H	1	Total	C	N	O	P	0	0
			36	22	4	9	1		
4	M	1	Total	C	N	O	P	0	0
			36	22	4	9	1		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N 5 3 2	0	0
5	A	1	Total C N 5 3 2	0	0
5	H	1	Total C N 5 3 2	0	0
5	M	1	Total C N 5 3 2	0	0

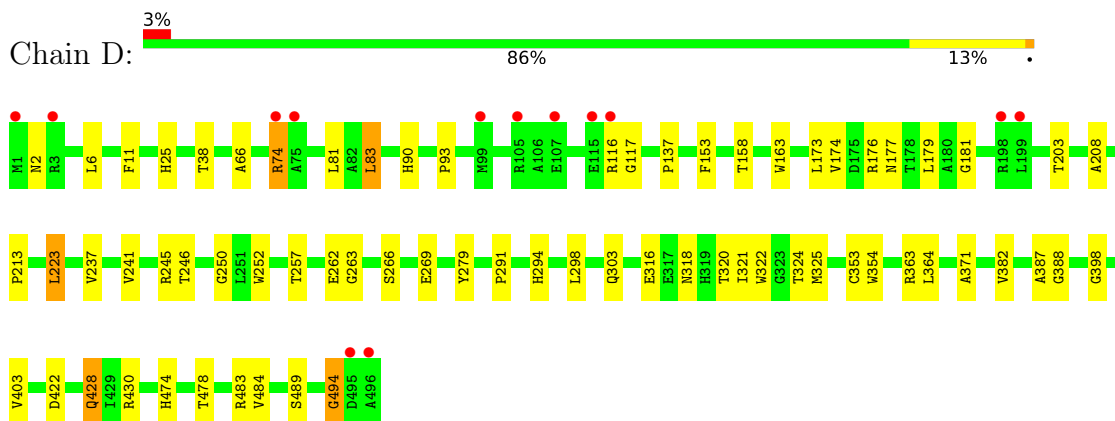
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	344	Total O 344 344	0	0
6	A	360	Total O 360 360	0	0
6	H	346	Total O 346 346	0	0
6	M	374	Total O 374 374	0	0

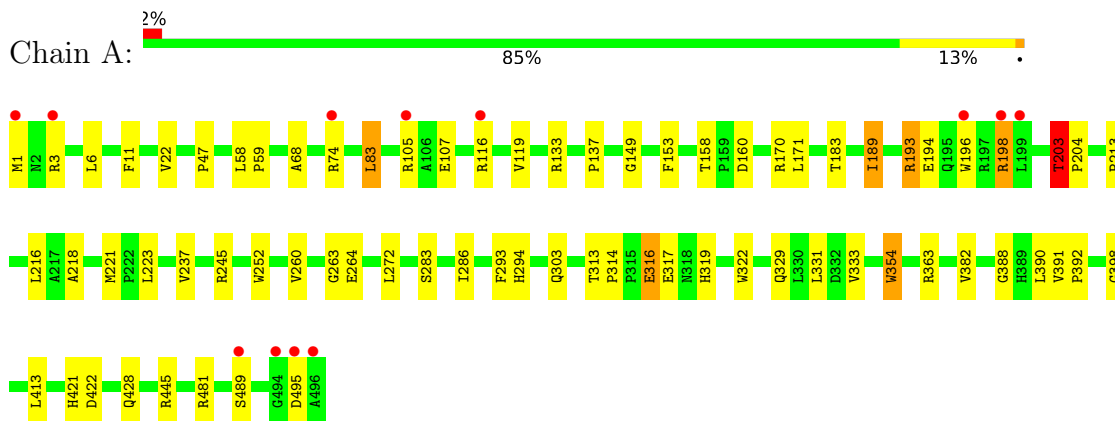
3 Residue-property plots

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

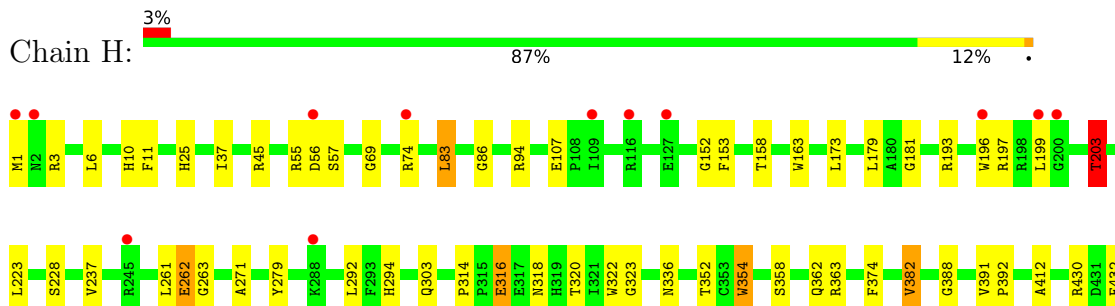
- Molecule 1: UbiD-like decarboxylase

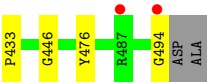


- Molecule 1: UbiD-like decarboxylase

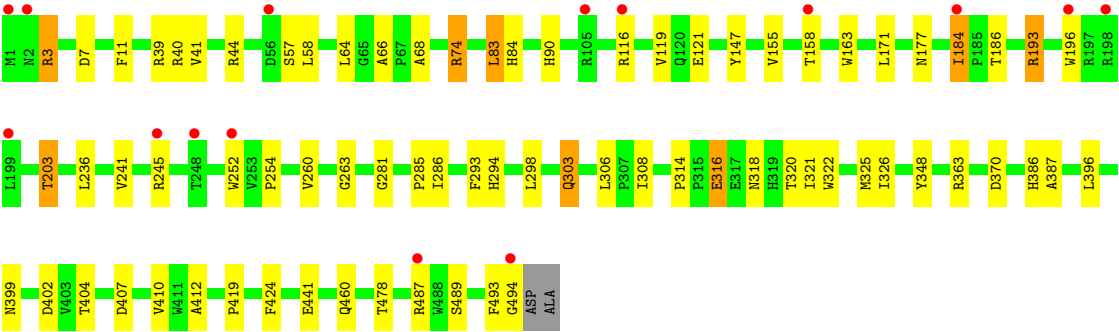
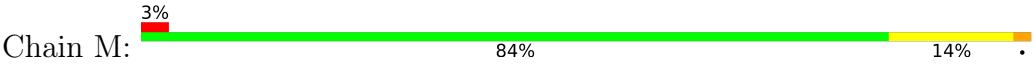


- Molecule 1: UbiD-like decarboxylase





● Molecule 1: UbiD-like decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.81Å 55.48Å 199.53Å 90.00° 99.92° 90.00°	Depositor
Resolution (Å)	53.64 – 1.65 53.64 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (53.64-1.65) 99.6 (53.64-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.235 0.212 , 0.241	Depositor DCC
R_{free} test set	14033 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16967	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 47.82 % 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 9.3937e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, 4LU, MN, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.48	21/3956 (0.5%)	1.25	13/5401 (0.2%)
1	D	1.46	15/3949 (0.4%)	1.29	19/5394 (0.4%)
1	H	1.46	18/3938 (0.5%)	1.25	7/5377 (0.1%)
1	M	1.46	24/3960 (0.6%)	1.27	14/5407 (0.3%)
All	All	1.46	78/15803 (0.5%)	1.26	53/21579 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	HIS	CA-C	9.21	1.60	1.52
1	M	66	ALA	C-O	-8.70	1.19	1.23
1	H	412	ALA	CA-C	-7.60	1.43	1.52
1	D	353	CYS	N-CA	7.28	1.55	1.46
1	M	460	GLN	N-CA	7.25	1.55	1.46

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	VAL	CA-C-N	-7.23	110.80	119.84
1	A	391	VAL	C-N-CA	-7.23	110.80	119.84
1	D	403	VAL	N-CA-C	6.54	121.06	112.76
1	H	203	THR	CB-CA-C	6.45	117.24	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	399	ASN	N-CA-C	6.23	120.57	113.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	476	TYR	Sidechain

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	3848	0	3770	34	0
1	D	3841	0	3754	29	0
1	H	3830	0	3752	32	0
1	M	3852	0	3777	36	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	H	1	0	0	0	0
2	M	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	H	1	0	0	0	0
3	M	1	0	0	0	0
4	A	36	0	28	9	0
4	D	36	0	28	10	0
4	H	36	0	27	4	0
4	M	36	0	27	3	0
5	A	5	0	5	9	0
5	D	5	0	5	7	0
5	H	5	0	4	2	0
5	M	5	0	4	1	0
6	A	360	0	0	12	0
6	D	344	0	0	6	0
6	H	346	0	0	12	0
6	M	374	0	0	14	0
All	All	16967	0	15181	157	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 5.

The worst 5 of 157 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)
4:D:503:4LU:C1	5:D:504:IMD:H2	1.49	1.42
1:M:407:ASP:HB2	6:M:864:HOH:O	1.21	1.32
1:D:158:THR:HB	6:D:846:HOH:O	1.20	1.31
1:H:158:THR:HB	6:H:827:HOH:O	1.15	1.30
4:D:503:4LU:C1	5:D:504:IMD:C2	2.13	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/496 (100%)	482 (98%)	12 (2%)	0	100	100
1	D	495/496 (100%)	483 (98%)	11 (2%)	1 (0%)	43	27
1	H	492/496 (99%)	475 (96%)	17 (4%)	0	100	100
1	M	494/496 (100%)	482 (98%)	12 (2%)	0	100	100
All	All	1975/1984 (100%)	1922 (97%)	52 (3%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	494	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/393 (100%)	379 (96%)	14 (4%)	31	9
1	D	391/393 (100%)	385 (98%)	6 (2%)	57	37
1	H	391/393 (100%)	379 (97%)	12 (3%)	35	12
1	M	394/393 (100%)	381 (97%)	13 (3%)	33	11
All	All	1569/1572 (100%)	1524 (97%)	45 (3%)	39	14

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	303	GLN
1	M	83	LEU
1	H	316	GLU
1	M	3	ARG
1	M	184[A]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	31	ASN
1	H	90	HIS
1	M	157	GLN
1	M	10	HIS
1	M	90	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
4	4LU	M	504	2,5,3	35,39,39	1.98	8 (22%)	44,62,62	2.43	13 (29%)
5	IMD	H	504	4	5,5,5	1.16	0	5,5,5	0.60	0
4	4LU	H	503	2,5,3	35,39,39	1.87	5 (14%)	44,62,62	2.61	17 (38%)
5	IMD	D	504	-	5,5,5	1.17	1 (20%)	5,5,5	0.54	0
4	4LU	D	503	2,3	35,39,39	1.76	8 (22%)	44,62,62	2.51	13 (29%)
5	IMD	A	504	-	5,5,5	0.79	0	5,5,5	0.56	0
5	IMD	M	501	4	5,5,5	0.70	0	5,5,5	0.54	0
4	4LU	A	503	2,3	35,39,39	1.80	9 (25%)	44,62,62	2.73	14 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4LU	M	504	2,5,3	-	3/18/30/30	0/4/4/4
5	IMD	H	504	4	-	-	0/1/1/1
4	4LU	H	503	2,5,3	-	3/18/30/30	0/4/4/4
5	IMD	D	504	-	-	-	0/1/1/1
4	4LU	D	503	2,3	-	3/18/30/30	0/4/4/4
5	IMD	A	504	-	-	-	0/1/1/1
5	IMD	M	501	4	-	-	0/1/1/1
4	4LU	A	503	2,3	-	3/18/30/30	0/4/4/4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	503	4LU	O2-C2	7.14	1.38	1.23
4	M	504	4LU	O2-C2	6.52	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	4LU	O2-C2	5.42	1.34	1.23
4	D	503	4LU	O4-C4	5.19	1.33	1.23
4	M	504	4LU	O4-C4	4.83	1.32	1.23

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	4LU	C12-C5-C3	-9.01	95.61	109.50
4	D	503	4LU	C12-C5-C3	-8.77	95.98	109.50
4	H	503	4LU	C5-C6-C5A	-7.79	112.97	121.48
4	M	504	4LU	C5-C6-C5A	-7.21	113.61	121.48
4	M	504	4LU	C12-C5-C3	-7.05	98.64	109.50

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	503	4LU	C2'-C1'-N10-C10
4	M	504	4LU	C2'-C3'-C4'-C5'
4	A	503	4LU	C2'-C3'-C4'-C5'
4	D	503	4LU	C2'-C3'-C4'-C5'
4	H	503	4LU	C2'-C3'-C4'-C5'

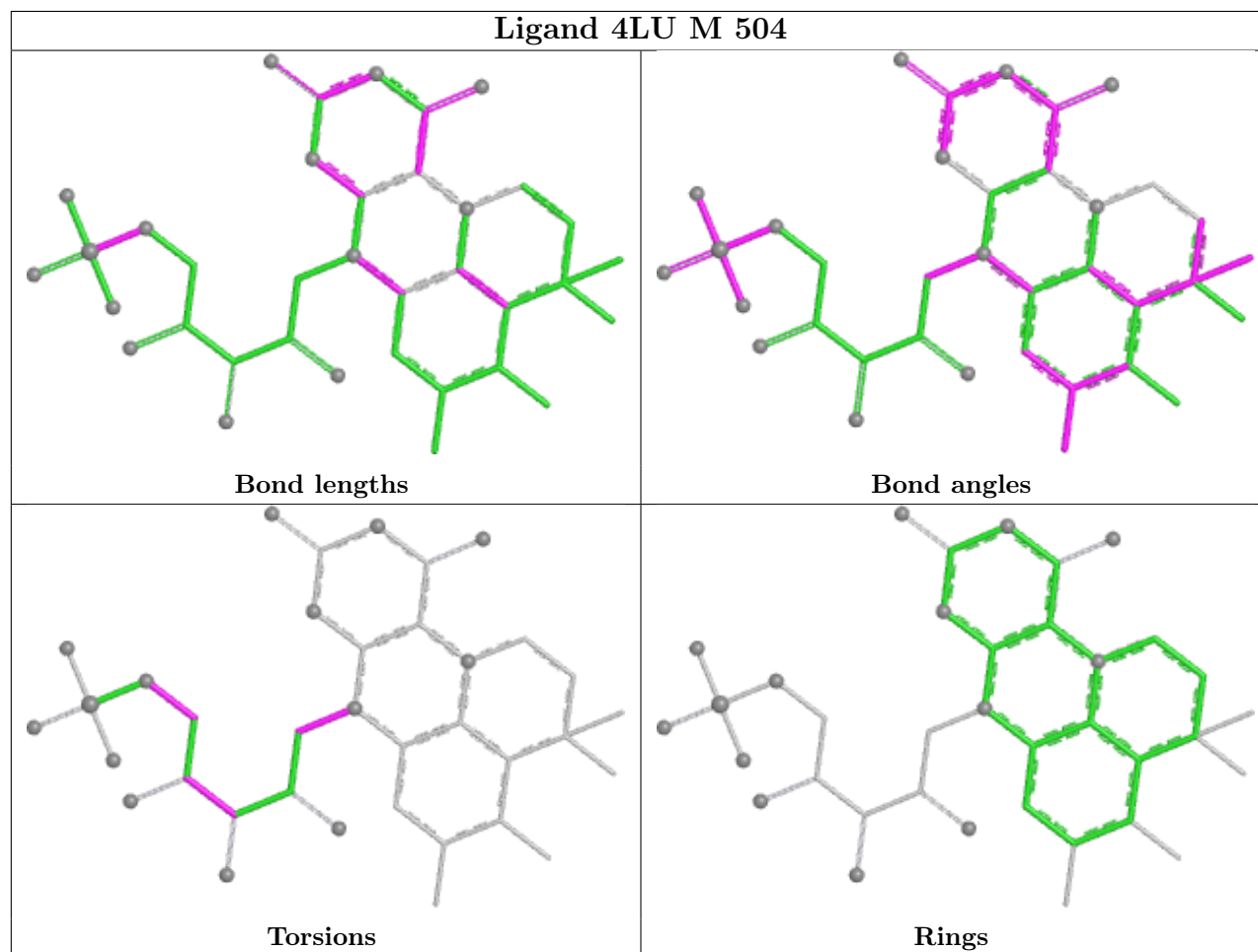
There are no ring outliers.

8 monomers are involved in 32 short contacts:

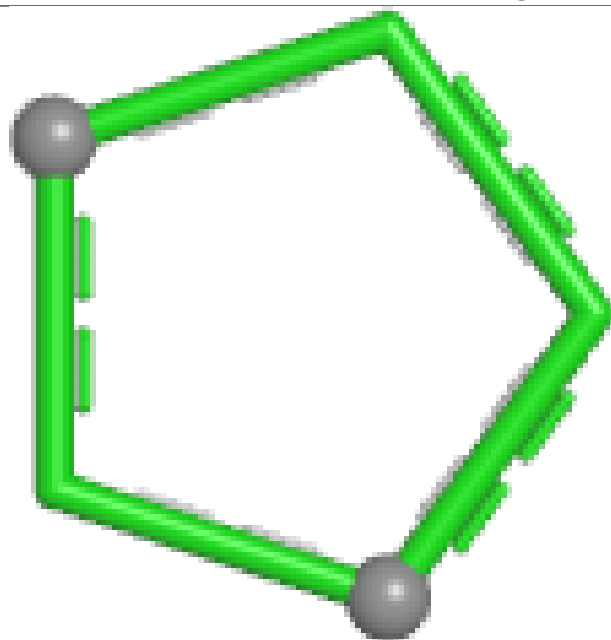
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	504	4LU	3	0
5	H	504	IMD	2	0
4	H	503	4LU	4	0
5	D	504	IMD	7	0
4	D	503	4LU	10	0
5	A	504	IMD	9	0
5	M	501	IMD	1	0
4	A	503	4LU	9	0

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.

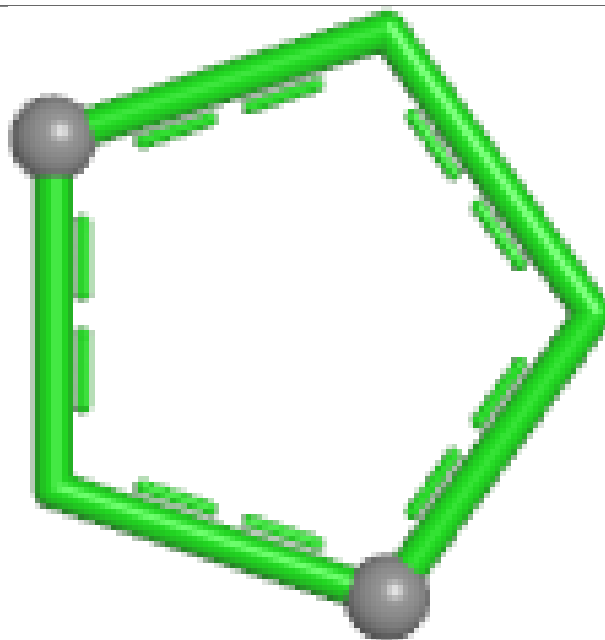
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



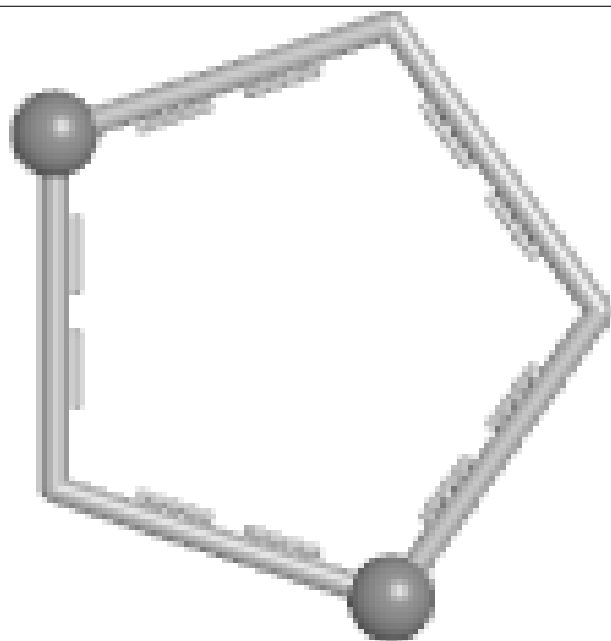
Ligand IMD H 504



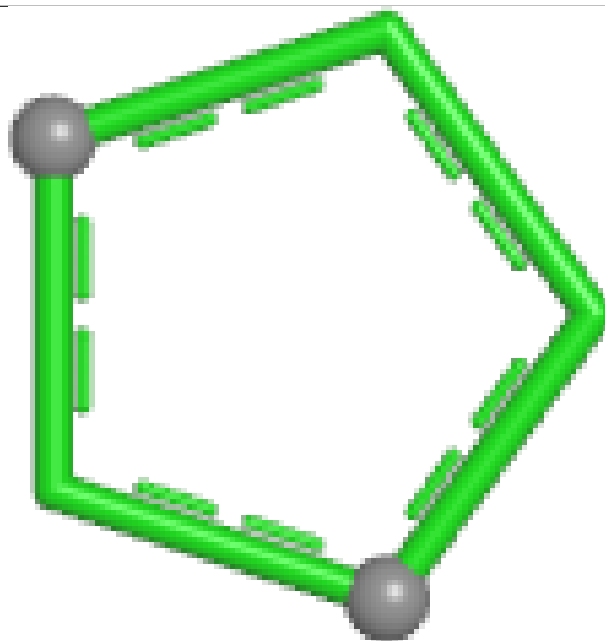
Bond lengths



Bond angles

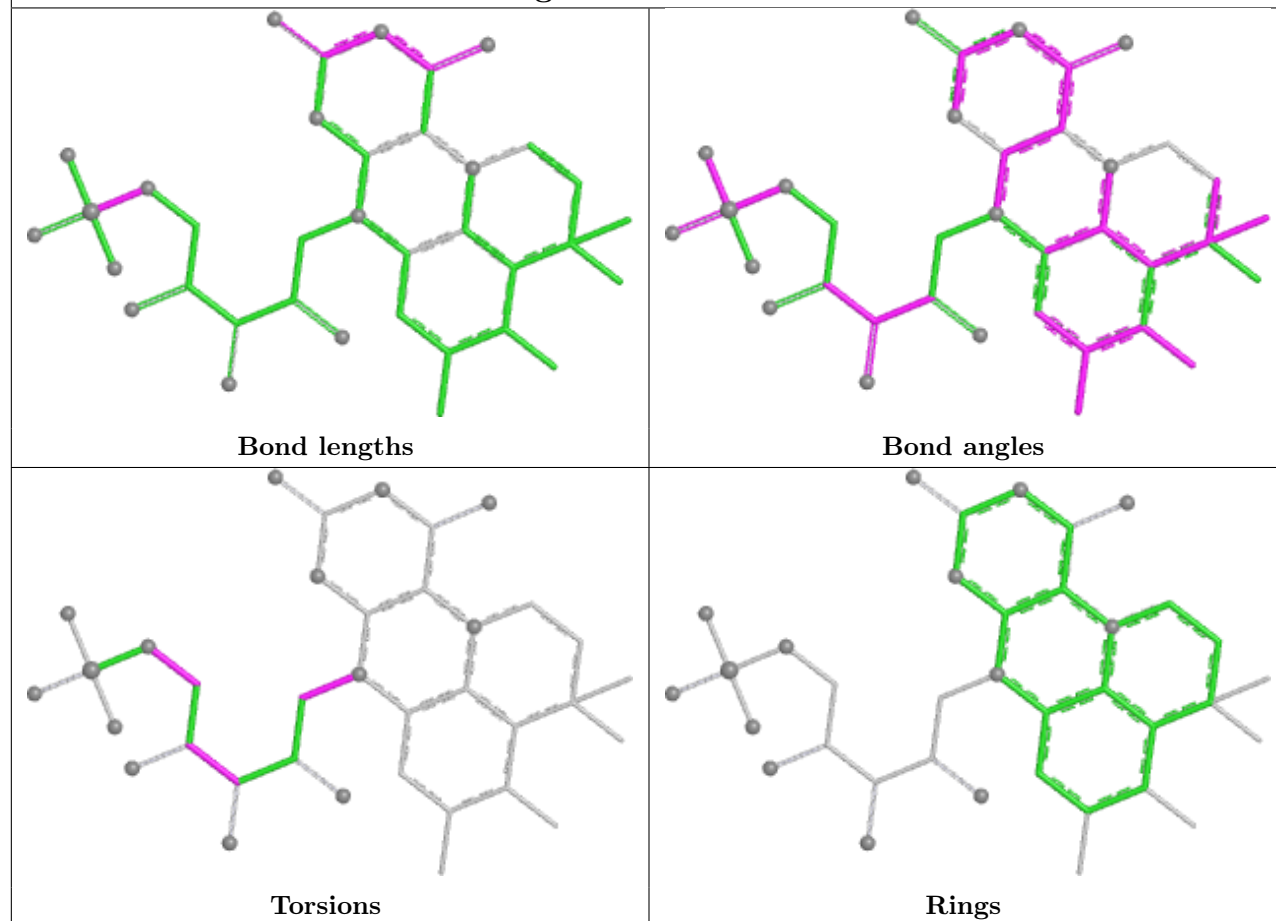


Torsions

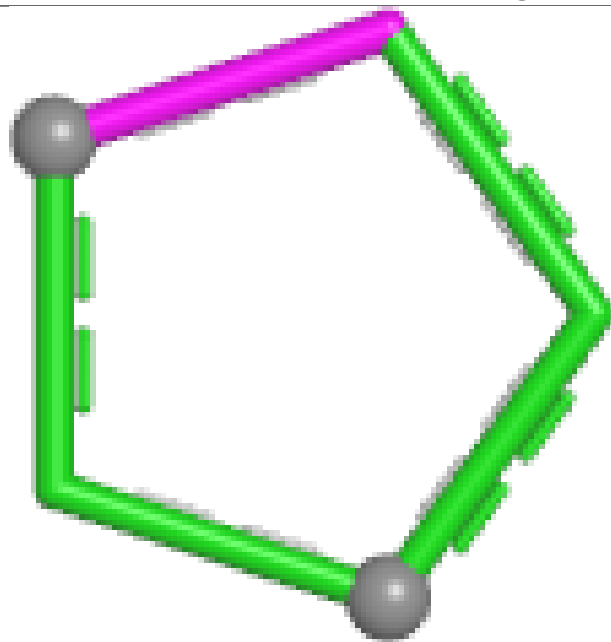


Rings

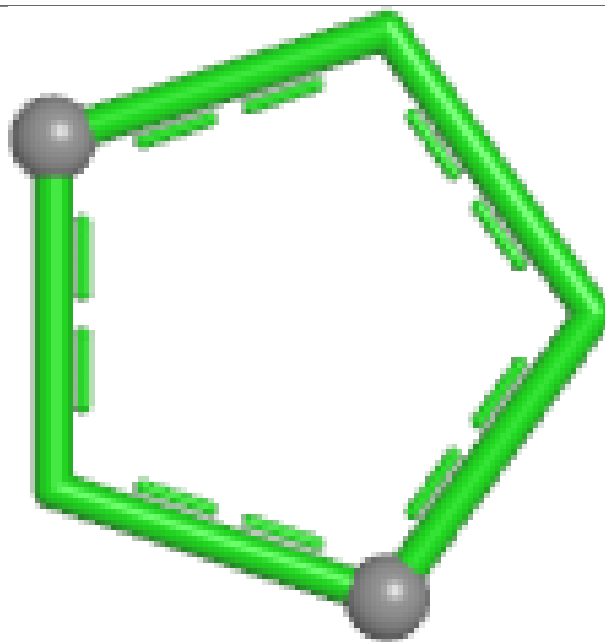
Ligand 4LU H 503



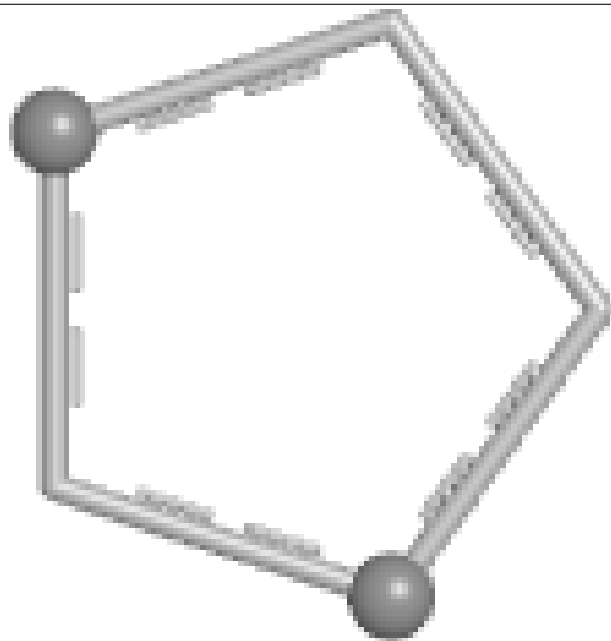
Ligand IMD D 504



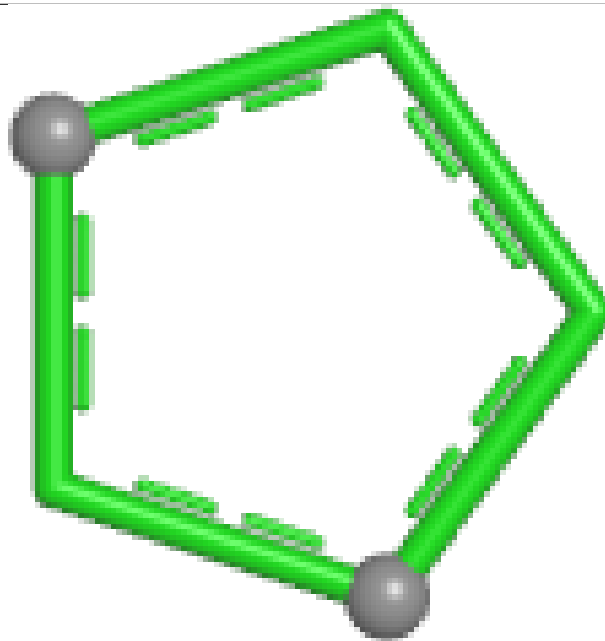
Bond lengths



Bond angles

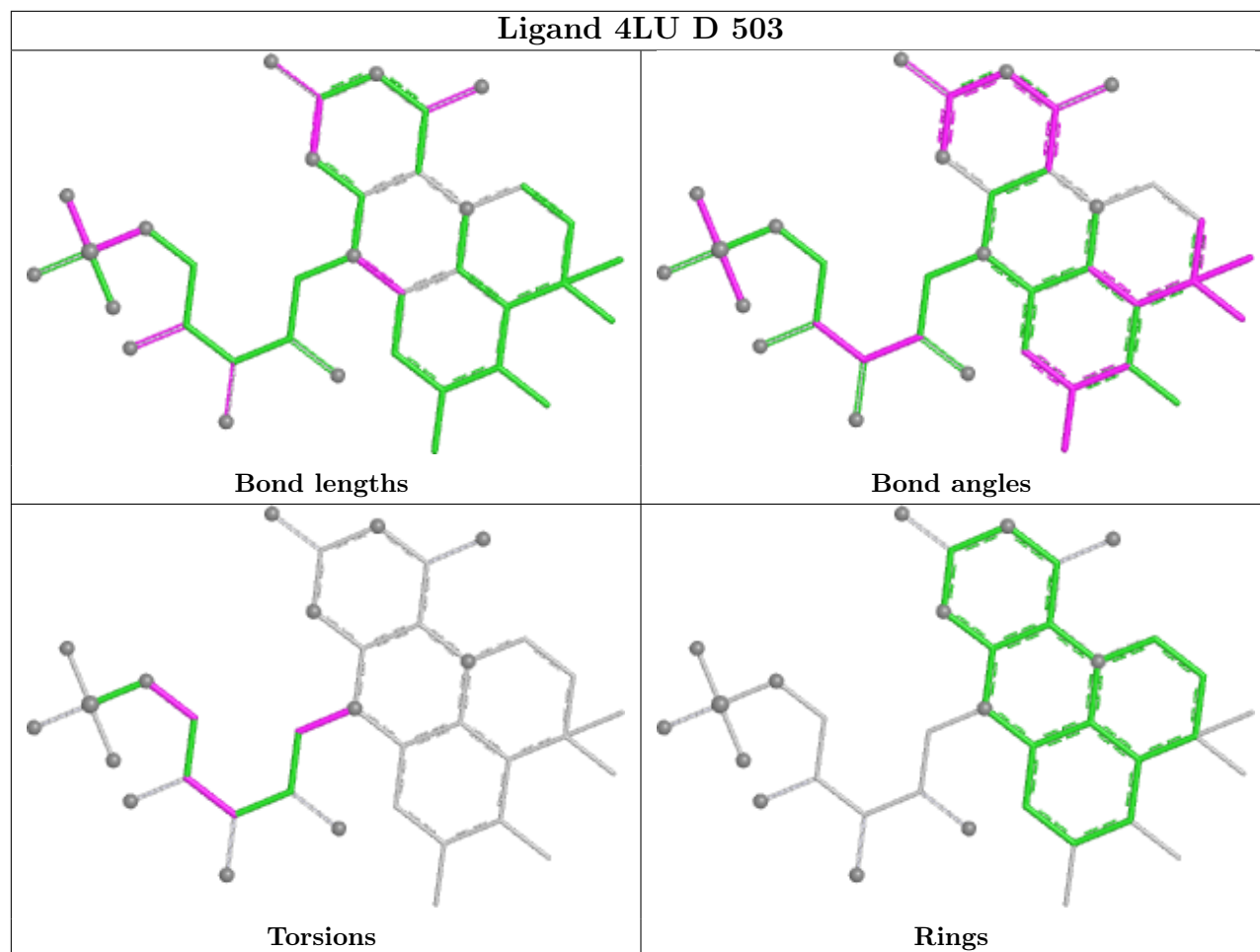


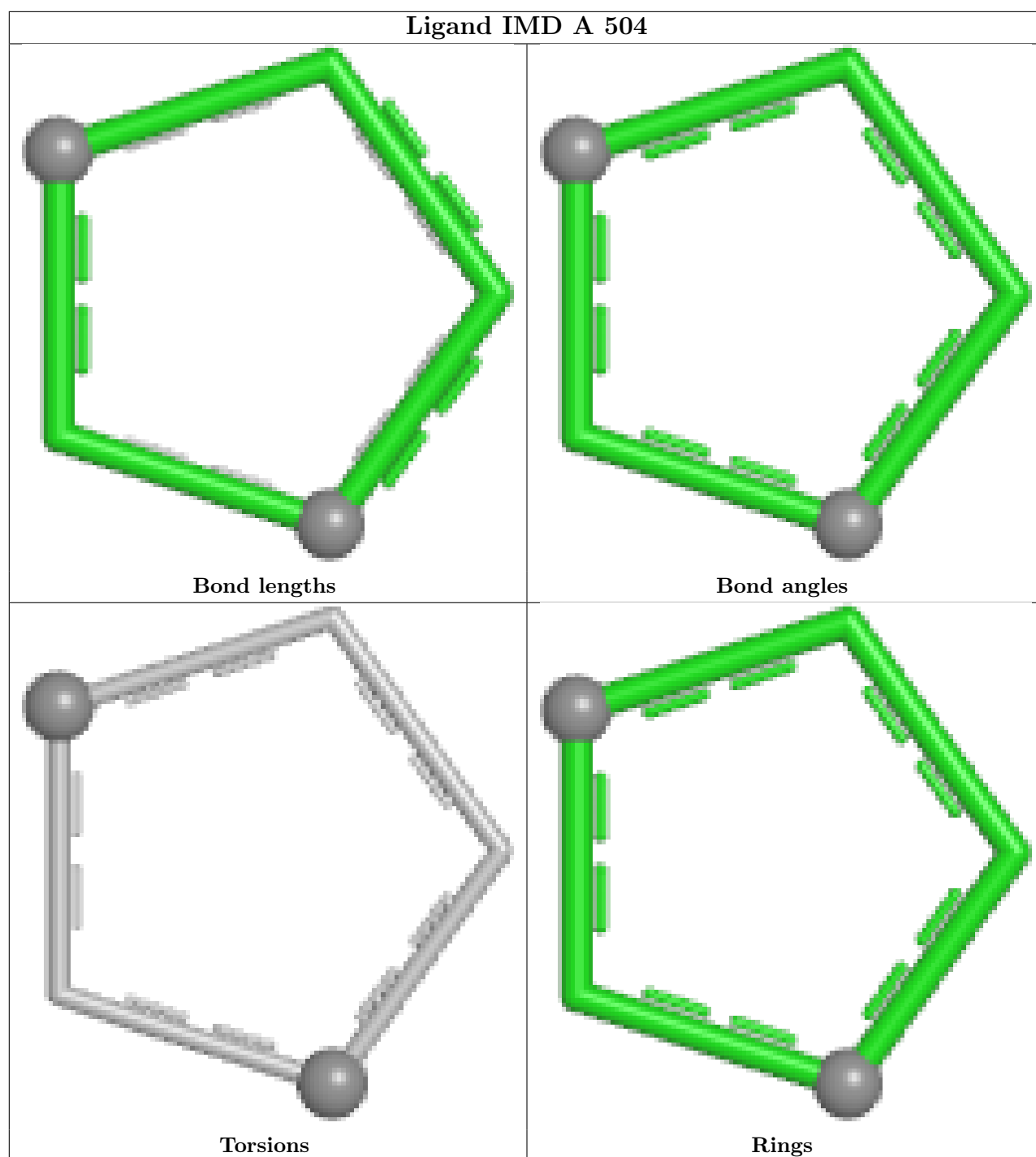
Torsions

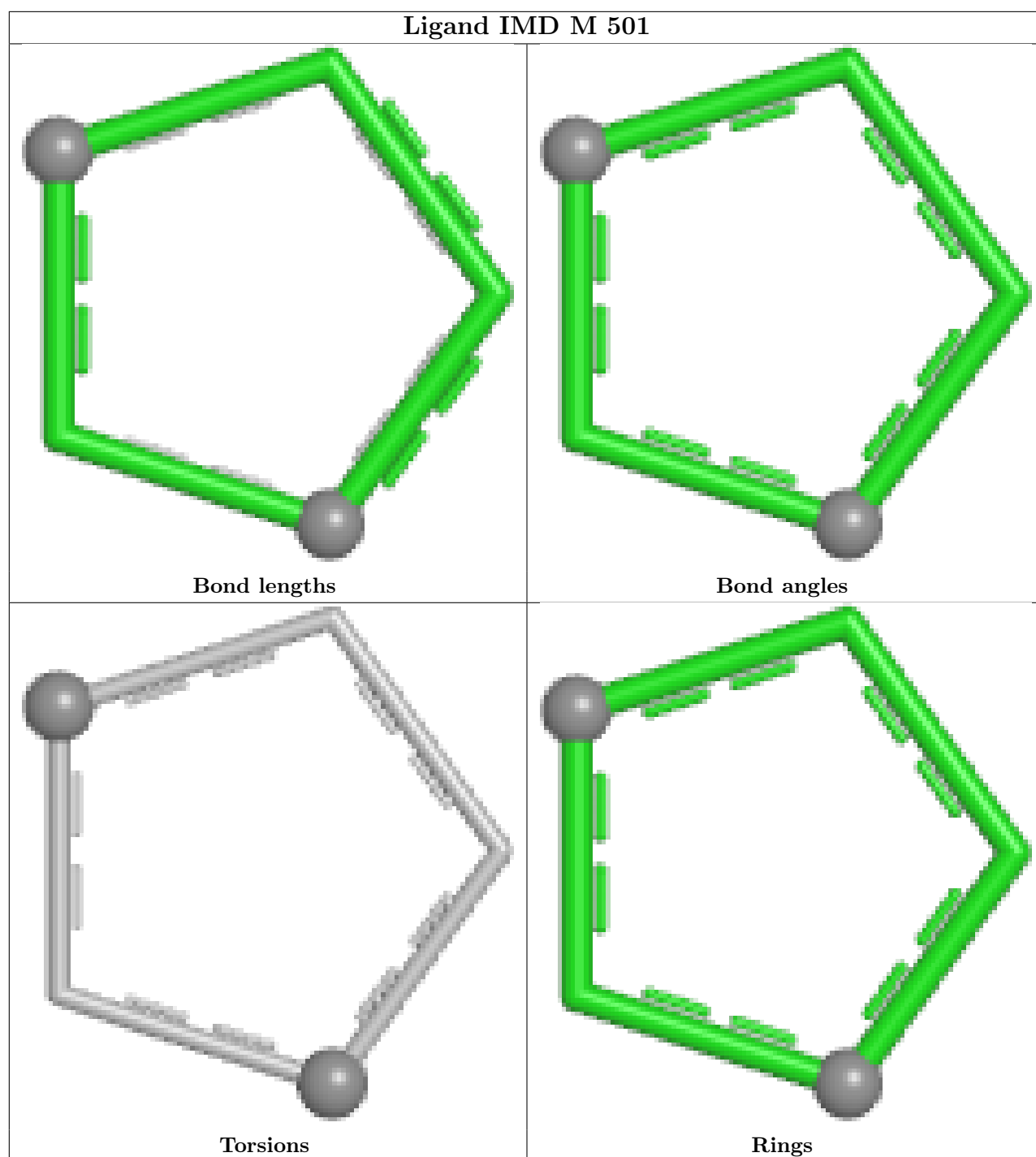


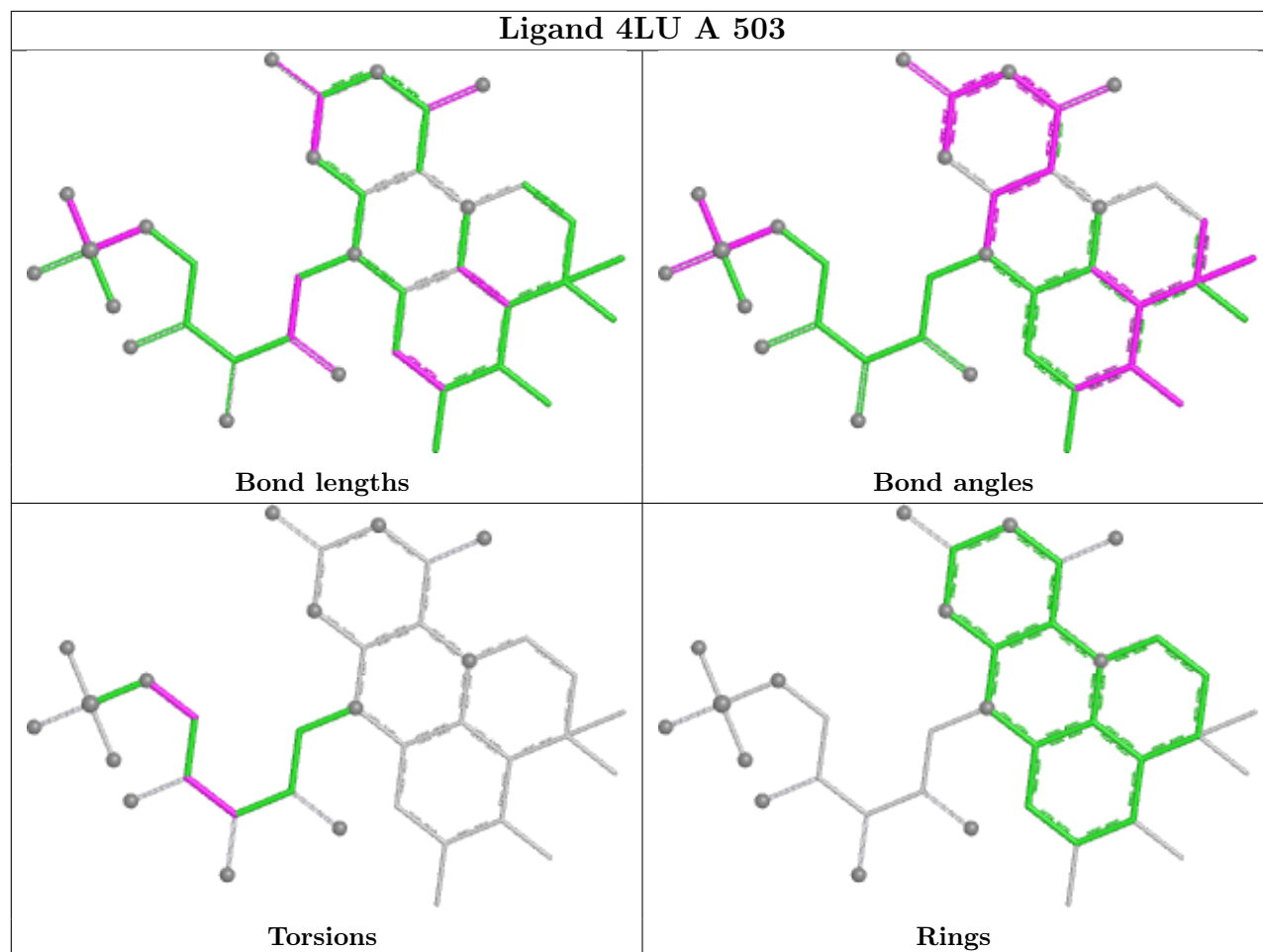
Rings

Ligand 4LU D 503









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	496/496 (100%)	0.06	12 (2%) 59 65	8, 16, 33, 51	0
1	D	496/496 (100%)	0.07	13 (2%) 57 62	9, 16, 32, 53	1 (0%)
1	H	494/496 (99%)	0.14	14 (2%) 55 60	9, 17, 34, 46	0
1	M	494/496 (99%)	0.12	15 (3%) 52 57	6, 17, 33, 53	2 (0%)
All	All	1980/1984 (99%)	0.10	54 (2%) 56 61	6, 17, 33, 53	3 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	199	LEU	4.7
1	M	2	ASN	4.1
1	M	116	ARG	3.8
1	M	198	ARG	3.6
1	H	494	GLY	3.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

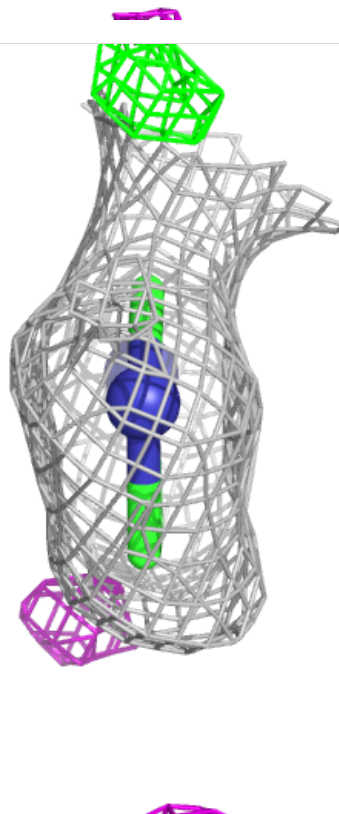
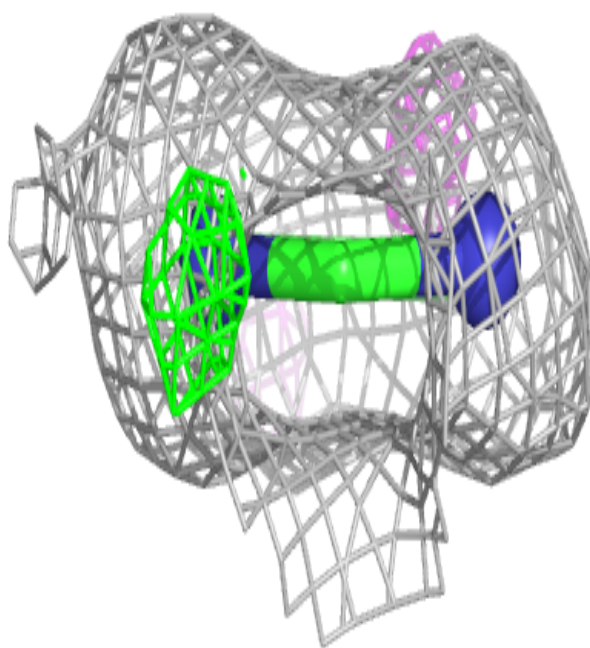
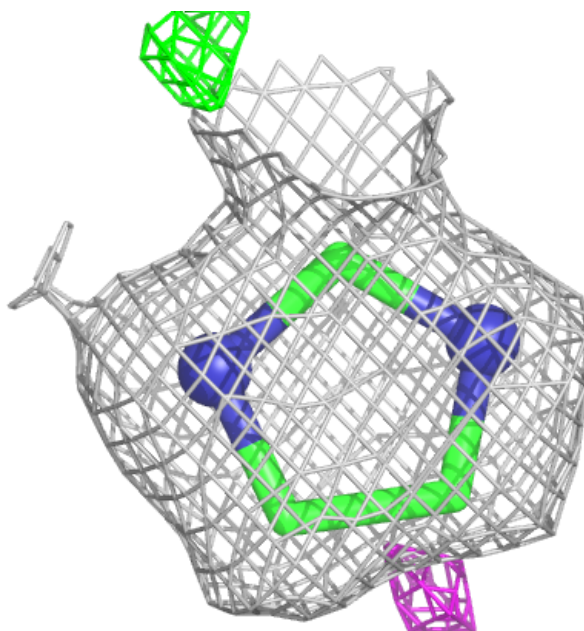
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IMD	H	504	5/5	0.91	0.15	19,20,21,22	0
5	IMD	A	504	5/5	0.93	0.17	23,25,27,28	0
5	IMD	D	504	5/5	0.93	0.12	20,22,23,23	0
5	IMD	M	501	5/5	0.94	0.09	17,19,20,20	0
4	4LU	D	503	36/36	0.96	0.07	10,14,19,20	0
4	4LU	A	503	36/36	0.96	0.07	10,14,19,21	0
4	4LU	H	503	36/36	0.96	0.07	10,15,20,22	0
4	4LU	M	504	36/36	0.96	0.07	12,15,20,20	0
2	MN	A	501	1/1	0.99	0.02	15,15,15,15	0
3	K	A	502	1/1	0.99	0.02	15,15,15,15	0
3	K	H	502	1/1	0.99	0.04	16,16,16,16	0
3	K	M	503	1/1	0.99	0.04	15,15,15,15	0
3	K	D	502	1/1	1.00	0.02	15,15,15,15	0
2	MN	D	501	1/1	1.00	0.02	14,14,14,14	0
2	MN	H	501	1/1	1.00	0.04	14,14,14,14	0
2	MN	M	502	1/1	1.00	0.03	15,15,15,15	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.

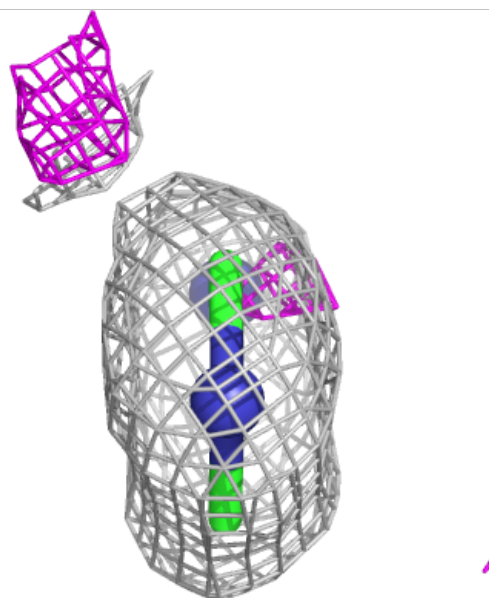
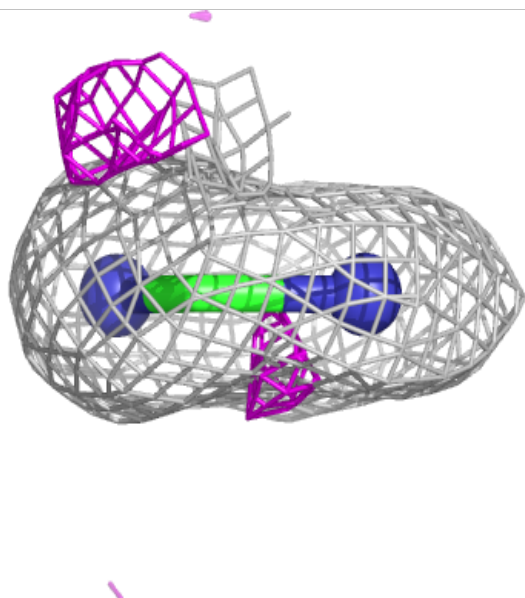
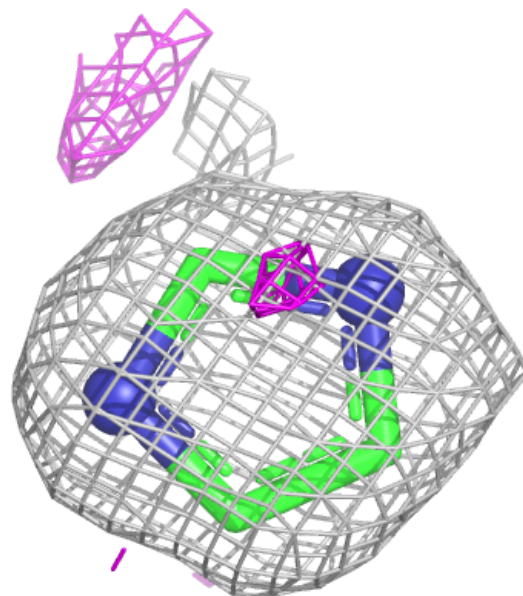
Electron density around IMD H 504:

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



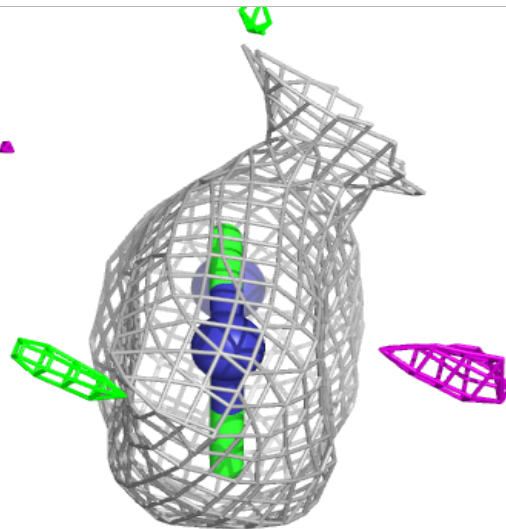
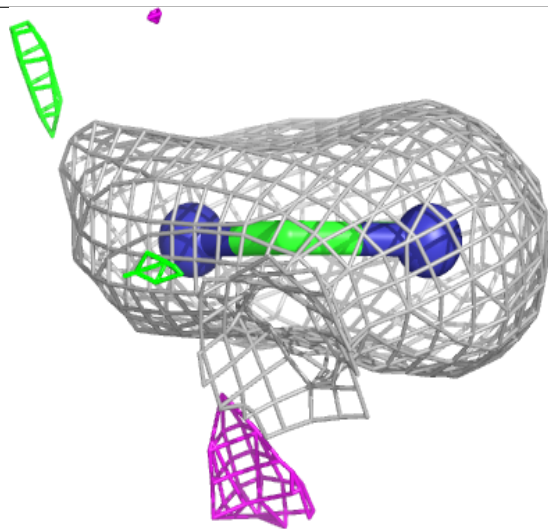
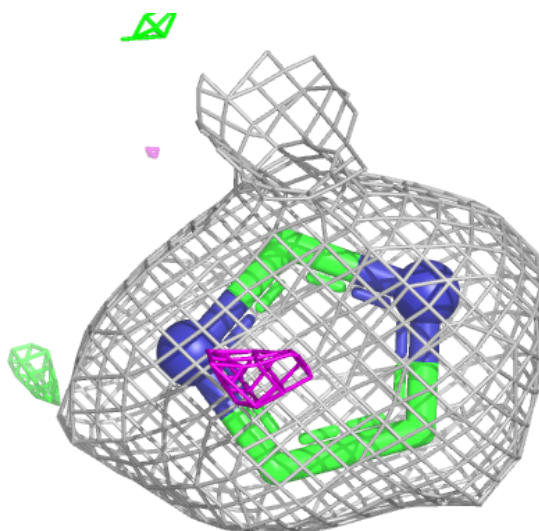
Electron density around IMD A 504:

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



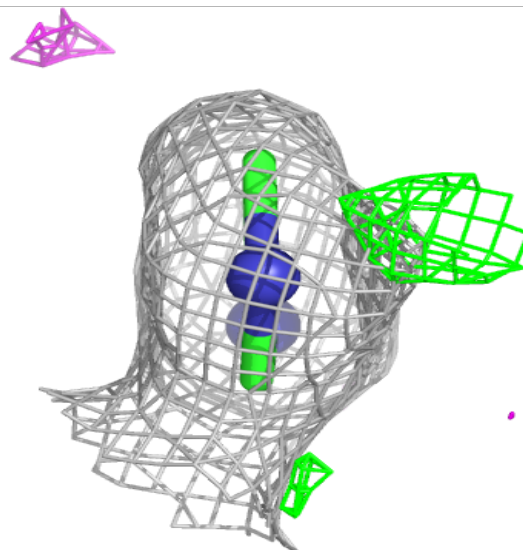
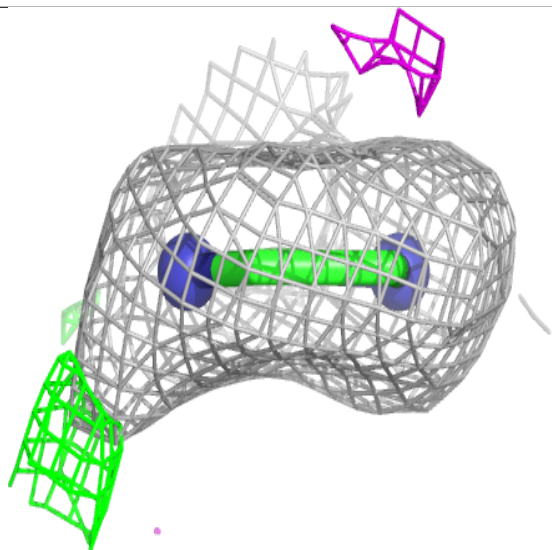
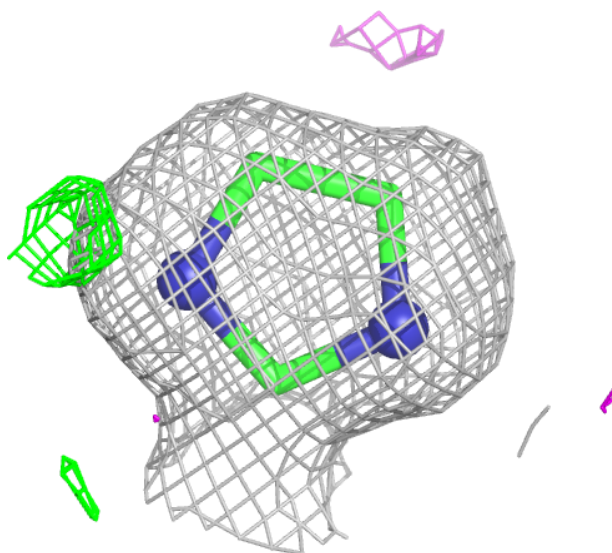
Electron density around IMD D 504:

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



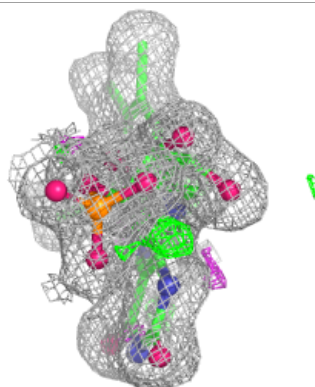
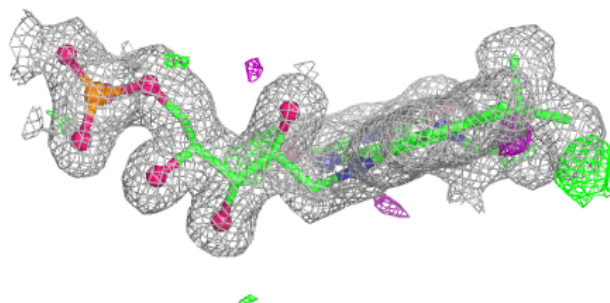
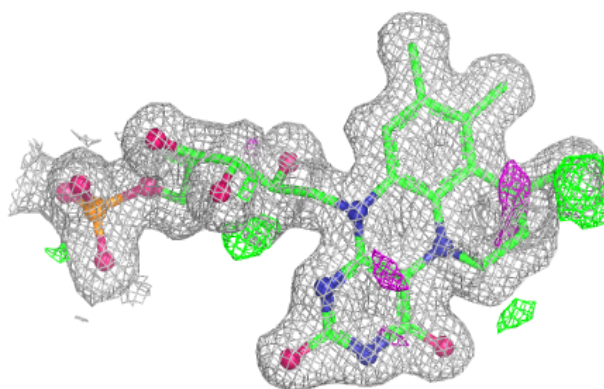
Electron density around IMD M 501:

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

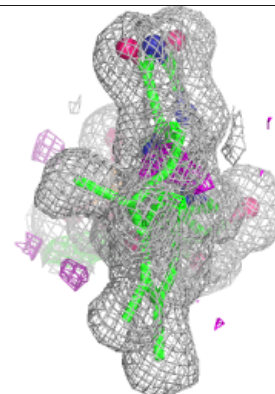
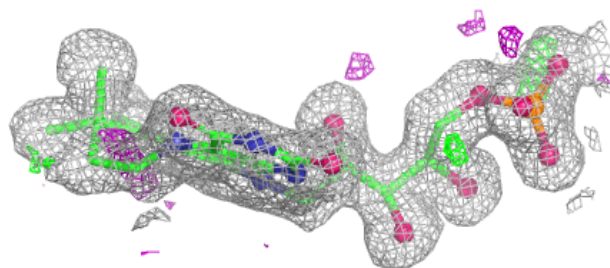
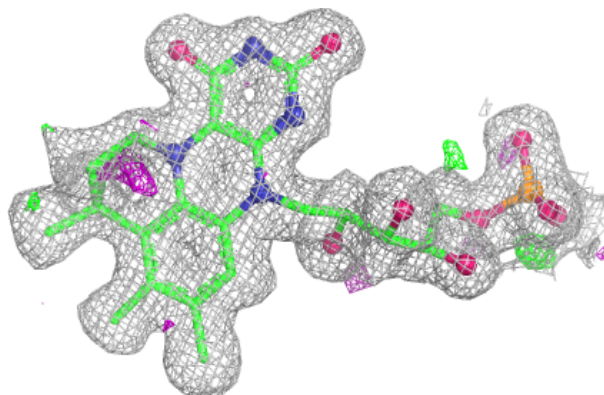


Electron density around 4LU D 503:

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

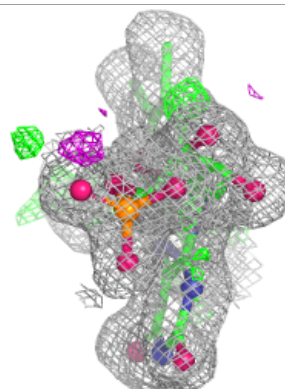
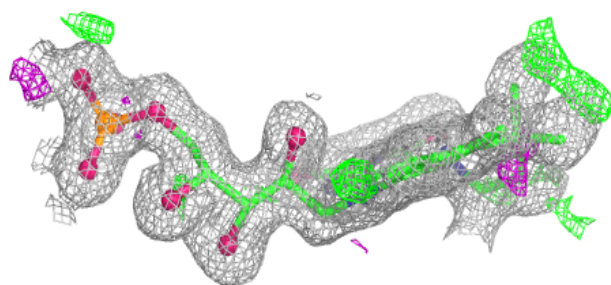
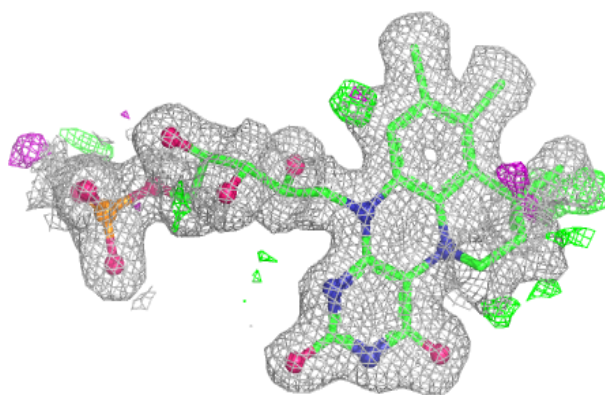
**Electron density around 4LU A 503:**

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

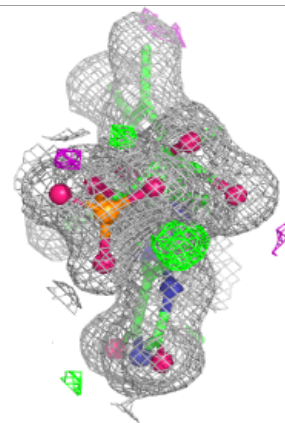
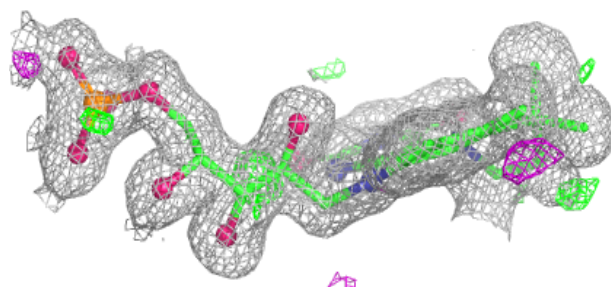
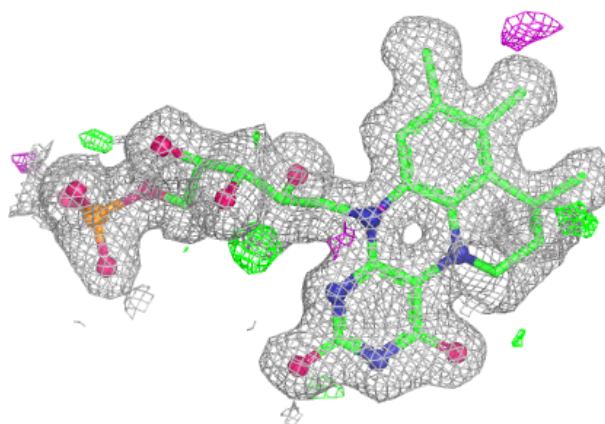


Electron density around 4LU H 503:

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

**Electron density around 4LU M 504:**

$2mF_o-DF_c$ (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.