Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 02:09 pm BST

PDB ID	:	7ABN
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

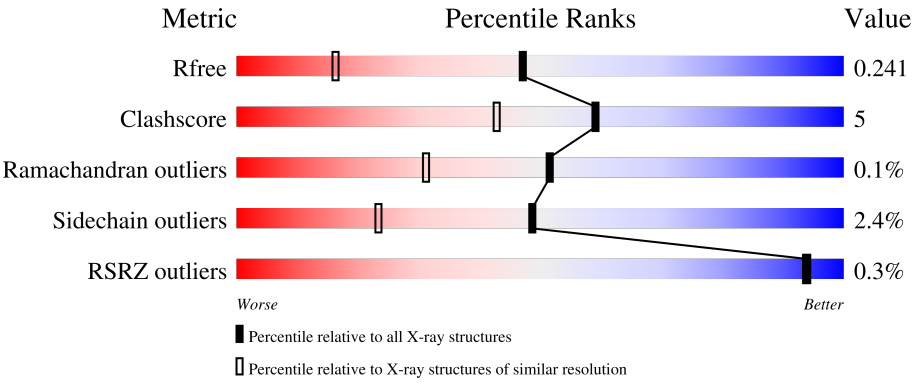
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (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 <=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	89% 10%
1	D	496	88% 11%
1	H	496	88% 11%
1	M	496	% 88% 10%

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

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			

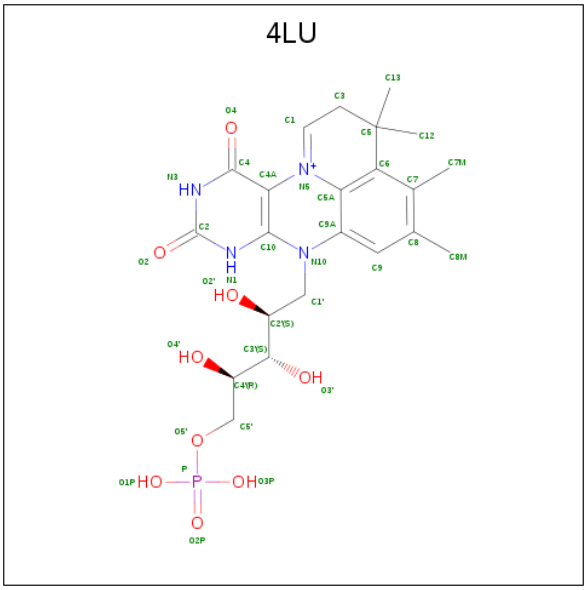
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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 (three-letter code: K) (formula: K).

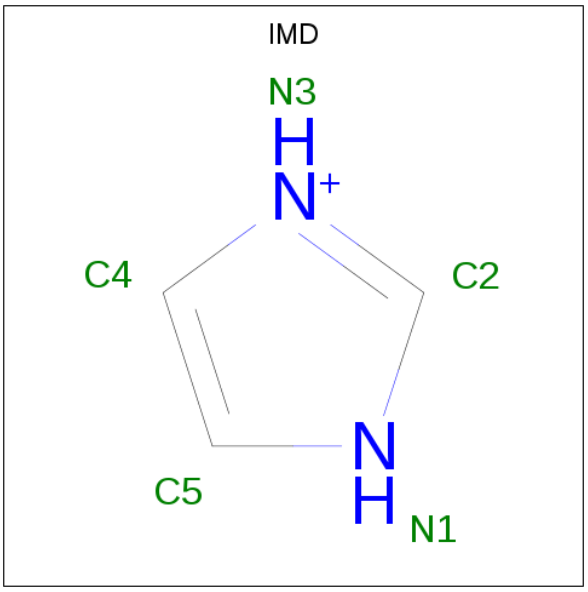
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	H	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

- 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-y l)-D-ribitol (three-letter code: 4LU) (formula: $C_{22}H_{30}N_4O_9P$) (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 (three-letter code: IMD) (formula: $C_3H_5N_2$) (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.

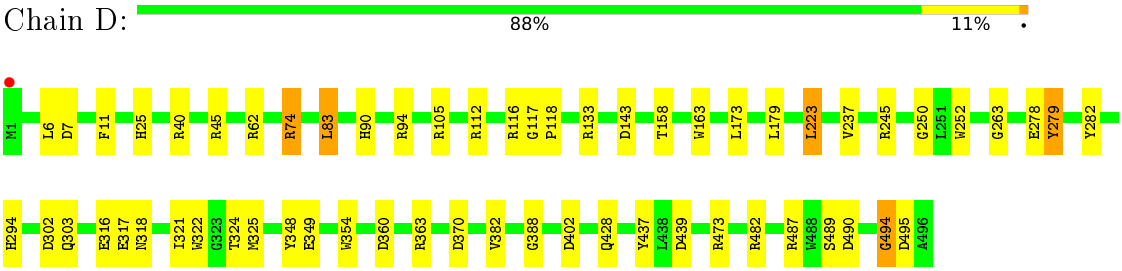
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	344	Total O 344 344	0	0
6	A	360	Total O 360 360	0	0
6	H	346	Total O 346 346	0	0
6	M	374	Total O 374 374	0	0

3 Residue-property plots (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.

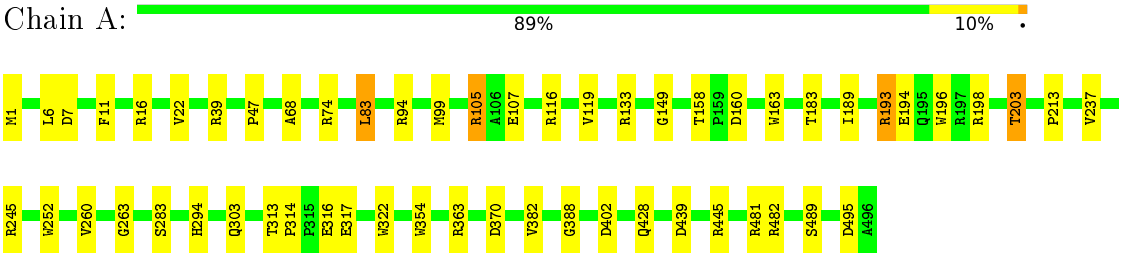
- Molecule 1: UbiD-like decarboxylase

Chain D:



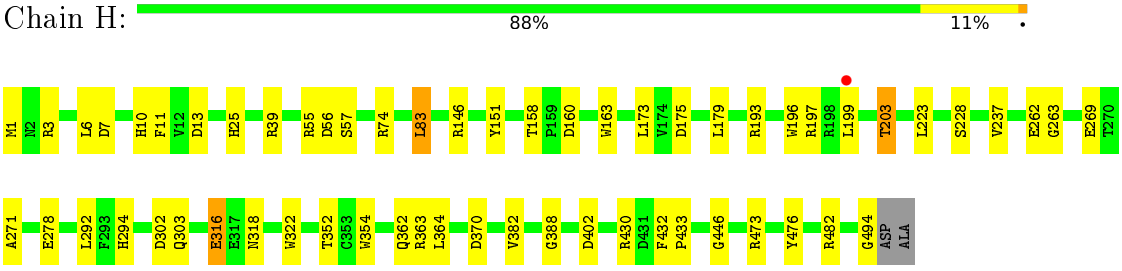
- Molecule 1: UbiD-like decarboxylase

Chain A:



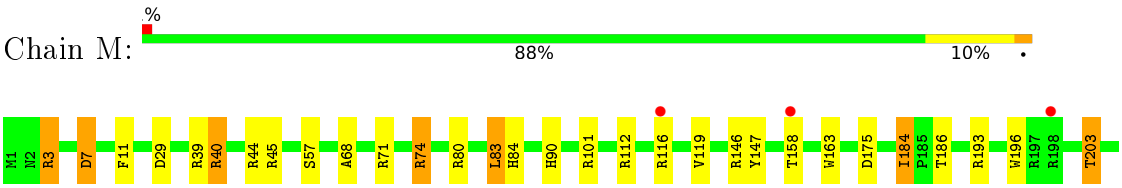
- Molecule 1: UbiD-like decarboxylase

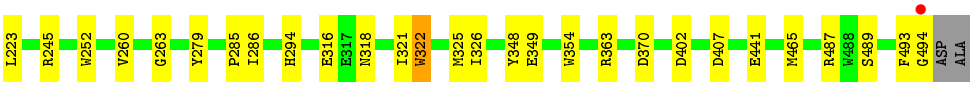
Chain H:



- Molecule 1: UbiD-like decarboxylase

Chain M:




L223
R245
W252
V260
G263
Y279
P285
I286
H294
E316
E317
N318
I321
W322
M325
I326
Y348
E349
W354
R363
D370
D402
D407
E441
M465
R487
W488
S489
F493
G494
ASP
ALA

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, K, 4LU, IMD

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	1.10	3/3956 (0.1%)	1.11	15/5401 (0.3%)
1	D	1.12	5/3949 (0.1%)	1.18	26/5394 (0.5%)
1	H	1.10	4/3938 (0.1%)	1.10	14/5377 (0.3%)
1	M	1.12	5/3960 (0.1%)	1.14	19/5407 (0.4%)
All	All	1.11	17/15803 (0.1%)	1.13	74/21579 (0.3%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	348	TYR	CG-CD2	7.35	1.48	1.39
1	A	283	SER	CA-CB	-7.14	1.42	1.52
1	M	147	TYR	CE1-CZ	-6.15	1.30	1.38
1	M	349	GLU	CD-OE1	-5.90	1.19	1.25
1	D	349	GLU	CD-OE2	5.75	1.31	1.25
1	M	279	TYR	CG-CD1	-5.59	1.31	1.39
1	H	269	GLU	CD-OE1	5.52	1.31	1.25
1	D	278	GLU	CD-OE1	5.49	1.31	1.25
1	M	322	TRP	CB-CG	5.38	1.59	1.50
1	A	163	TRP	CB-CG	5.33	1.59	1.50
1	H	278	GLU	CG-CD	5.29	1.59	1.51
1	D	437	TYR	CE1-CZ	-5.26	1.31	1.38
1	H	352	THR	CB-OG1	5.26	1.53	1.43
1	D	317	GLU	CD-OE2	5.21	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	GLY	C-O	-5.19	1.15	1.23
1	H	151	TYR	CE1-CZ	5.14	1.45	1.38
1	D	279	TYR	CD2-CE2	5.09	1.47	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	39	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	D	370	ASP	CB-CG-OD1	10.97	128.17	118.30
1	M	370	ASP	CB-CG-OD1	10.52	127.77	118.30
1	D	402	ASP	CB-CG-OD1	9.62	126.96	118.30
1	H	39	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	D	223	LEU	CB-CG-CD1	9.08	126.43	111.00
1	A	105	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	H	370	ASP	CB-CG-OD1	8.68	126.11	118.30
1	D	473	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	M	39	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	A	370	ASP	CB-CG-OD1	8.50	125.95	118.30
1	D	370	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	D	112	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	481	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	A	402	ASP	CB-CG-OD1	7.62	125.16	118.30
1	M	45	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	105	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	M	80	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	D	143	ASP	CB-CG-OD1	7.27	124.84	118.30
1	H	39	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	M	370	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	M	112	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	105	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	370	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	A	94	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	481	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	M	45	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	D	45	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	302	ASP	CB-CG-OD1	6.51	124.16	118.30
1	D	482	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	M	71	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	M	402	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	348	TYR	CB-CG-CD1	6.36	124.81	121.00
1	M	29	ASP	CB-CG-OD1	6.29	123.96	118.30
1	H	278	GLU	OE1-CD-OE2	-6.25	115.80	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	348	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	D	439	ASP	CB-CG-OD2	6.18	123.86	118.30
1	M	7	ASP	CB-CG-OD1	6.17	123.85	118.30
1	M	465	MET	CG-SD-CE	6.03	109.85	100.20
1	D	62	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	H	364	LEU	CB-CG-CD2	-5.99	100.83	111.00
1	D	302	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	D	40	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	99	MET	CG-SD-CE	5.85	109.56	100.20
1	H	160	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	482	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	105	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	H	473	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	7	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	39	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	45	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	H	482	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	H	175	ASP	CB-CG-OD1	5.54	123.28	118.30
1	D	94	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	M	175	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	487	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	D	7	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	133	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	M	40	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	482	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	M	223	LEU	CB-CG-CD1	5.30	120.00	111.00
1	H	13	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	H	402	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	360	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	M	101	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	282	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	16	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	439	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	193	ARG	CG-CD-NE	-5.17	100.95	111.80
1	H	302	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	H	146	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	D	490	ASP	CB-CG-OD1	5.08	122.87	118.30
1	H	7	ASP	CB-CG-OD1	5.01	122.81	118.30
1	M	146	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	31	0
1	D	3841	0	3754	26	0
1	H	3830	0	3752	30	0
1	M	3852	0	3777	34	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	10	0
4	D	36	0	28	8	0
4	H	36	0	27	3	0
4	M	36	0	27	2	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	11	0
6	M	374	0	0	14	0
All	All	16967	0	15181	144	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.

All (144) 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
1:M:158:THR:HB	6:M:871:HOH:O	1.05	1.23
1:A:428:GLN:HG2	6:A:610:HOH:O	1.36	1.20
4:A:503:4LU:C1	5:A:504:IMD:C2	2.20	1.19
4:A:503:4LU:C1	5:A:504:IMD:H2	1.73	1.19
1:D:303:GLN:HG3	6:D:894:HOH:O	1.45	1.13
1:H:228:SER:HB3	6:H:647:HOH:O	1.48	1.13
4:D:503:4LU:H6	5:D:504:IMD:H2	1.11	1.08
4:M:504:4LU:H14	4:M:504:4LU:H13	1.42	1.02
4:D:503:4LU:H14	4:D:503:4LU:H13	1.42	1.00
4:D:503:4LU:H6	5:D:504:IMD:C2	1.83	0.95
1:H:193:ARG:HA	1:H:203:THR:HG21	1.48	0.92
4:A:503:4LU:C3	5:A:504:IMD:H2	2.00	0.92
4:H:503:4LU:H14	4:H:503:4LU:H13	1.53	0.90
4:A:503:4LU:H6	5:A:504:IMD:C2	2.04	0.88
4:A:503:4LU:H6	5:A:504:IMD:N1	1.90	0.86
1:M:193:ARG:HA	1:M:203:THR:HG21	1.58	0.85
1:A:193:ARG:HA	1:A:203:THR:HG21	1.57	0.85
4:A:503:4LU:H14	4:A:503:4LU:H13	1.59	0.84
4:A:503:4LU:H9	5:A:504:IMD:H2	1.61	0.81
4:D:503:4LU:H14	4:D:503:4LU:C12	2.12	0.76
4:M:504:4LU:H14	4:M:504:4LU:C12	2.16	0.74
1:A:428:GLN:CG	6:A:610:HOH:O	2.12	0.72
4:H:503:4LU:H14	4:H:503:4LU:C12	2.21	0.69
1:H:3:ARG:HD2	6:H:602:HOH:O	1.93	0.67
4:D:503:4LU:C3	5:D:504:IMD:H2	2.24	0.67
1:A:133:ARG:NH1	6:A:603:HOH:O	2.26	0.66
1:D:363:ARG:HD2	6:D:850:HOH:O	1.96	0.66
1:M:487:ARG:NH1	6:M:603:HOH:O	2.26	0.66
1:H:3:ARG:CD	6:H:602:HOH:O	2.44	0.66
1:M:196:TRP:CD1	1:M:203:THR:HB	2.32	0.65
1:M:3:ARG:CD	6:M:602:HOH:O	2.44	0.65
1:M:74:ARG:HB3	1:M:74:ARG:CZ	2.27	0.64
1:A:22:VAL:HG23	1:A:47:PRO:HB2	1.78	0.64
4:A:503:4LU:H6	5:A:504:IMD:HN1	1.62	0.63
1:A:322:TRP:CH2	5:A:504:IMD:H4	2.34	0.63
1:M:263:GLY:HA3	1:M:294:HIS:O	1.98	0.62
4:A:503:4LU:H14	4:A:503:4LU:C12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:TRP:CZ3	5:D:504:IMD:H5	2.34	0.61
1:A:303:GLN:NE2	6:A:604:HOH:O	2.33	0.60
1:M:322:TRP:CZ3	5:M:501:IMD:H4	2.37	0.60
1:M:158:THR:HG22	1:M:163:TRP:H	1.68	0.59
1:D:245:ARG:HG3	1:D:252:TRP:CZ2	2.37	0.58
1:H:196:TRP:CD1	1:H:203:THR:HB	2.38	0.58
4:A:503:4LU:C1	5:A:504:IMD:N1	2.56	0.57
1:D:6:LEU:HD21	1:D:237:VAL:HG21	1.86	0.57
1:D:245:ARG:HG3	1:D:252:TRP:CE2	2.40	0.57
1:M:3:ARG:HD3	6:M:602:HOH:O	2.04	0.56
1:H:6:LEU:HD21	1:H:237:VAL:HG21	1.88	0.56
1:D:321:ILE:O	1:D:325:MET:HG2	2.06	0.55
1:H:228:SER:CB	6:H:647:HOH:O	2.24	0.55
1:H:74:ARG:CZ	1:H:74:ARG:HB3	2.36	0.55
1:H:263:GLY:HA3	1:H:294:HIS:O	2.07	0.55
1:A:445:ARG:NH1	6:A:602:HOH:O	2.12	0.55
1:A:6:LEU:HD21	1:A:237:VAL:HG21	1.88	0.54
1:A:196:TRP:CD1	1:A:203:THR:HB	2.43	0.54
1:M:7:ASP:OD2	6:M:602:HOH:O	2.19	0.54
1:H:322:TRP:CZ3	5:H:504:IMD:H5	2.44	0.53
1:A:107:GLU:HG2	6:A:621:HOH:O	2.09	0.52
1:M:321:ILE:O	1:M:325:MET:HG2	2.10	0.52
1:A:263:GLY:HA3	1:A:294:HIS:O	2.09	0.52
1:H:382:VAL:O	1:H:388:GLY:HA3	2.08	0.52
1:D:263:GLY:HA3	1:D:294:HIS:O	2.10	0.51
1:A:74:ARG:CZ	1:A:74:ARG:HB3	2.40	0.51
1:M:90:HIS:HD2	6:M:879:HOH:O	1.92	0.51
1:H:56:ASP:O	6:H:601:HOH:O	2.18	0.51
1:H:158:THR:HG22	1:H:163:TRP:H	1.76	0.51
4:H:503:4LU:N5	4:H:503:4LU:H5	2.26	0.51
1:A:303:GLN:NE2	6:A:608:HOH:O	2.40	0.50
1:A:445:ARG:NH2	6:A:609:HOH:O	2.41	0.50
1:M:3:ARG:HD2	6:M:602:HOH:O	2.09	0.50
1:A:1:MET:N	6:A:601:HOH:O	2.05	0.50
1:H:173:LEU:HA	1:H:179:LEU:HD23	1.92	0.50
1:D:11:PHE:CD1	1:D:83:LEU:HD13	2.47	0.50
6:D:772:HOH:O	1:H:25:HIS:HE1	1.94	0.50
1:D:116:ARG:HD3	1:D:117:GLY:N	2.27	0.49
1:H:203:THR:HG22	6:H:682:HOH:O	2.12	0.49
1:M:11:PHE:CD1	1:M:83:LEU:HD13	2.47	0.49
1:M:493:PHE:O	1:M:494:GLY:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:TRP:CE3	5:D:504:IMD:H5	2.47	0.49
1:M:245:ARG:HG2	1:M:252:TRP:CZ2	2.47	0.48
1:A:194:GLU:HG3	1:A:198:ARG:NH1	2.28	0.48
1:D:428:GLN:HA	1:D:428:GLN:OE1	2.14	0.48
1:A:11:PHE:CD1	1:A:83:LEU:HD13	2.48	0.48
1:A:119:VAL:HG21	1:A:260:VAL:HG23	1.95	0.48
1:H:1:MET:N	6:H:607:HOH:O	2.47	0.47
1:M:441:GLU:HB3	6:M:952:HOH:O	2.14	0.47
1:A:363:ARG:HD2	6:A:896:HOH:O	2.12	0.47
1:D:382:VAL:O	1:D:388:GLY:HA3	2.16	0.46
1:H:193:ARG:HG3	1:H:203:THR:CG2	2.46	0.46
1:M:68:ALA:HB2	1:M:84:HIS:CE1	2.52	0.45
1:D:173:LEU:HA	1:D:179:LEU:HD23	1.98	0.45
1:M:441:GLU:CG	6:M:952:HOH:O	2.64	0.45
1:D:158:THR:HG22	1:D:163:TRP:H	1.82	0.44
1:M:441:GLU:HG2	6:M:952:HOH:O	2.17	0.44
1:D:303:GLN:NE2	6:D:606:HOH:O	2.50	0.44
1:A:1:MET:CA	6:A:601:HOH:O	2.59	0.44
1:A:203:THR:HG22	6:A:801:HOH:O	2.17	0.44
1:D:74:ARG:CZ	1:D:74:ARG:HB3	2.46	0.44
1:D:324:THR:HG22	1:D:325:MET:HE2	2.00	0.44
1:A:193:ARG:HA	1:A:203:THR:CG2	2.39	0.43
1:A:428:GLN:HA	1:A:428:GLN:OE1	2.18	0.43
1:A:382:VAL:O	1:A:388:GLY:HA3	2.18	0.43
1:A:183:THR:HG22	1:A:189:ILE:HD13	2.00	0.43
1:M:40:ARG:HG2	1:M:44:ARG:HD3	2.01	0.43
1:M:322:TRP:O	1:M:326:ILE:HG13	2.19	0.43
1:M:158:THR:CG2	1:M:163:TRP:H	2.31	0.43
1:M:184[A]:ILE:HD11	1:M:186:THR:OG1	2.18	0.43
1:D:245:ARG:CZ	1:D:250:GLY:HA2	2.49	0.43
4:D:503:4LU:N5	4:D:503:4LU:H5	2.34	0.43
1:A:245:ARG:HG3	1:A:252:TRP:CH2	2.54	0.43
1:H:430:ARG:HG3	1:H:446:GLY:O	2.19	0.43
1:M:119:VAL:HG21	1:M:260:VAL:HG23	2.01	0.43
1:D:25:HIS:HD2	6:H:902:HOH:O	2.01	0.43
1:M:318:ASN:O	1:M:322:TRP:HB3	2.19	0.43
1:M:441:GLU:HG2	6:M:868:HOH:O	2.20	0.42
1:H:494:GLY:C	6:H:619:HOH:O	2.58	0.42
1:M:184[A]:ILE:HG23	6:M:639:HOH:O	2.20	0.42
1:A:68:ALA:HB3	1:A:317:GLU:HG3	2.00	0.42
1:A:313:THR:HA	1:A:314:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:THR:CG2	1:D:163:TRP:H	2.32	0.41
1:H:3:ARG:HG2	1:H:10:HIS:CG	2.55	0.41
1:H:196:TRP:HB2	1:H:203:THR:HG22	2.02	0.41
1:H:363:ARG:HD2	6:H:879:HOH:O	2.19	0.41
1:D:489:SER:HB2	1:D:494:GLY:HA2	2.02	0.41
1:H:432:PHE:CD1	1:H:433:PRO:HD2	2.55	0.41
1:M:441:GLU:CB	6:M:952:HOH:O	2.68	0.41
1:A:158:THR:HG21	1:A:160:ASP:OD1	2.21	0.41
1:H:271:ALA:HB2	1:H:292:LEU:HD21	2.03	0.41
1:H:322:TRP:CE3	5:H:504:IMD:H5	2.56	0.41
1:H:11:PHE:CD2	1:H:83:LEU:HD13	2.55	0.41
1:D:279:TYR:HB2	1:D:318:ASN:HB3	2.02	0.41
1:D:428:GLN:OE1	1:D:428:GLN:CA	2.67	0.41
1:H:197:ARG:O	1:H:197:ARG:HG2	2.21	0.41
1:H:316:GLU:OE2	1:H:318:ASN:N	2.49	0.41
1:D:90:HIS:HB2	6:D:892:HOH:O	2.20	0.41
1:M:193:ARG:HA	1:M:203:THR:CG2	2.40	0.41
1:M:285:PRO:C	1:M:286:ILE:HD13	2.42	0.40
1:M:363:ARG:HE	1:M:363:ARG:HB3	1.69	0.40
1:A:158:THR:CG2	1:A:160:ASP:OD1	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/496 (100%)	482 (98%)	12 (2%)	0	100	100
1	D	495/496 (100%)	483 (98%)	11 (2%)	1 (0%)	47	28
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%)	51	31

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%)	384 (98%)	9 (2%)	50	25
1	D	391/393 (100%)	384 (98%)	7 (2%)	59	36
1	H	391/393 (100%)	380 (97%)	11 (3%)	43	18
1	M	394/393 (100%)	382 (97%)	12 (3%)	41	15
All	All	1569/1572 (100%)	1530 (98%)	39 (2%)	49	22

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	ARG
1	D	83	LEU
1	D	118	PRO
1	D	223	LEU
1	D	316	GLU
1	D	354	TRP
1	D	495	ASP
1	A	83	LEU
1	A	105	ARG
1	A	116	ARG
1	A	203	THR
1	A	213	PRO
1	A	316	GLU
1	A	354	TRP
1	A	489	SER
1	A	495	ASP
1	H	55	ARG
1	H	57	SER
1	H	83	LEU

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Mol	Chain	Res	Type
1	H	199	LEU
1	H	203	THR
1	H	223	LEU
1	H	262	GLU
1	H	303	GLN
1	H	316	GLU
1	H	354	TRP
1	H	362	GLN
1	M	3	ARG
1	M	57	SER
1	M	74	ARG
1	M	83	LEU
1	M	116	ARG
1	M	184[A]	ILE
1	M	184[B]	ILE
1	M	203	THR
1	M	316[A]	GLU
1	M	316[B]	GLU
1	M	354	TRP
1	M	489	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	303	GLN
1	A	10	HIS
1	A	303	GLN
1	H	10	HIS
1	H	25	HIS
1	H	90	HIS
1	M	10	HIS
1	M	25	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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	IMD	A	504	-	3,5,5	0.54	0	4,5,5	0.42	0
4	4LU	H	503	3,2,5	32,39,39	1.63	7 (21%)	41,62,62	3.00	16 (39%)
4	4LU	A	503	3,2	32,39,39	1.64	8 (25%)	41,62,62	3.18	14 (34%)
5	IMD	M	501	4	3,5,5	0.46	0	4,5,5	0.62	0
5	IMD	D	504	-	3,5,5	1.18	0	4,5,5	0.59	0
4	4LU	D	503	3,2	32,39,39	1.98	9 (28%)	41,62,62	3.01	17 (41%)
4	4LU	M	504	3,2,5	32,39,39	1.85	5 (15%)	41,62,62	3.05	14 (34%)
5	IMD	H	504	4	3,5,5	0.87	0	4,5,5	0.52	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	IMD	A	504	-	-	-	0/1/1/1
4	4LU	H	503	3,2,5	-	2/18/30/30	0/3/4/4
4	4LU	A	503	3,2	-	3/18/30/30	0/3/4/4
5	IMD	M	501	4	-	-	0/1/1/1
5	IMD	D	504	-	-	-	0/1/1/1

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

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	504	4LU	C9A-N10	6.69	1.47	1.38
4	D	503	4LU	C9A-N10	6.28	1.47	1.38
4	M	504	4LU	C4-C4A	4.45	1.49	1.41
4	H	503	4LU	C4-C4A	4.23	1.48	1.41
4	D	503	4LU	C4-N3	3.93	1.39	1.33
4	D	503	4LU	O4-C4	3.52	1.33	1.24
4	A	503	4LU	P-O5'	3.25	1.70	1.60
4	M	504	4LU	O4-C4	3.25	1.32	1.24
4	H	503	4LU	C9A-N10	2.95	1.42	1.38
4	A	503	4LU	C9A-N10	2.95	1.42	1.38
4	A	503	4LU	P-O1P	-2.90	1.43	1.54
4	H	503	4LU	C2-N3	-2.76	1.32	1.38
4	H	503	4LU	O4-C4	2.76	1.31	1.24
4	A	503	4LU	O4-C4	2.75	1.31	1.24
4	D	503	4LU	C10-N1	2.75	1.36	1.33
4	M	504	4LU	P-O5'	2.72	1.69	1.60
4	D	503	4LU	O3'-C3'	2.70	1.49	1.43
4	A	503	4LU	C10-N1	2.68	1.36	1.33
4	A	503	4LU	C4-C4A	2.56	1.45	1.41
4	A	503	4LU	C2-N1	-2.48	1.33	1.38
4	D	503	4LU	P-O1P	-2.45	1.45	1.54
4	D	503	4LU	P-O5'	2.45	1.68	1.60
4	H	503	4LU	C6-C5A	-2.38	1.39	1.43
4	M	504	4LU	C2-N3	-2.31	1.33	1.38
4	D	503	4LU	C2-N1	-2.25	1.33	1.38
4	H	503	4LU	C1'-N10	-2.18	1.46	1.48
4	A	503	4LU	O2'-C2'	2.16	1.47	1.43
4	D	503	4LU	O4'-C4'	2.09	1.47	1.43
4	H	503	4LU	P-O5'	2.04	1.66	1.60

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	503	4LU	C4A-N5-C5A	-11.08	112.95	120.99
4	M	504	4LU	C1'-N10-C9A	9.15	125.49	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	504	4LU	C4A-N5-C5A	-9.10	114.39	120.99
4	A	503	4LU	C12-C5-C6	8.74	120.27	111.72
4	A	503	4LU	C4A-N5-C5A	-8.54	114.80	120.99
4	D	503	4LU	C12-C5-C6	8.17	119.72	111.72
4	A	503	4LU	C12-C5-C3	-8.07	95.61	109.60
4	D	503	4LU	C4A-N5-C5A	-7.89	115.27	120.99
4	D	503	4LU	C12-C5-C3	-7.86	95.98	109.60
4	A	503	4LU	C1'-N10-C9A	6.93	123.74	118.29
4	M	504	4LU	C12-C5-C3	-6.32	98.64	109.60
4	H	503	4LU	C5A-C9A-N10	-6.30	115.38	120.43
4	M	504	4LU	C4-C4A-C10	-6.29	115.79	119.95
4	H	503	4LU	C4-C4A-C10	-6.26	115.81	119.95
4	D	503	4LU	C4-C4A-C10	-5.48	116.33	119.95
4	A	503	4LU	O3P-P-O5'	-4.79	93.98	106.73
4	D	503	4LU	C9A-N10-C10	-4.64	115.84	121.91
4	M	504	4LU	C9A-N10-C10	-4.59	115.89	121.91
4	A	503	4LU	C9A-N10-C10	-4.38	116.17	121.91
4	H	503	4LU	C12-C5-C6	4.34	115.97	111.72
4	D	503	4LU	C4-N3-C2	4.33	118.80	115.14
4	H	503	4LU	C4-N3-C2	4.31	118.78	115.14
4	M	504	4LU	C5A-C9A-N10	-4.27	117.01	120.43
4	H	503	4LU	C12-C5-C3	-4.26	102.22	109.60
4	H	503	4LU	C8M-C8-C9	-4.06	110.64	120.34
4	M	504	4LU	C4-N3-C2	4.00	118.52	115.14
4	M	504	4LU	C12-C5-C6	3.96	115.59	111.72
4	D	503	4LU	C13-C5-C6	-3.92	107.88	111.72
4	H	503	4LU	C8M-C8-C7	3.91	127.26	121.17
4	A	503	4LU	O1P-P-O3P	3.83	122.26	107.64
4	A	503	4LU	C4-N3-C2	3.82	118.37	115.14
4	H	503	4LU	C7M-C7-C8	-3.80	112.72	119.71
4	A	503	4LU	C8-C7-C6	3.46	122.47	119.43
4	D	503	4LU	C12-C5-C13	3.35	116.19	108.67
4	D	503	4LU	C4A-C4-N3	-3.35	118.85	123.43
4	A	503	4LU	C4A-C4-N3	-3.32	118.90	123.43
4	A	503	4LU	C4-C4A-C10	-3.28	117.78	119.95
4	H	503	4LU	O3P-P-O5'	-3.23	98.13	106.73
4	M	504	4LU	C1'-N10-C10	-3.19	115.55	118.41
4	A	503	4LU	C7M-C7-C8	-3.03	114.13	119.71
4	H	503	4LU	C9A-N10-C10	-2.95	118.04	121.91
4	M	504	4LU	O1P-P-O2P	2.90	122.03	110.68
4	M	504	4LU	O3P-P-O5'	-2.88	99.06	106.73
4	D	503	4LU	C7-C6-C5A	-2.84	116.23	119.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	503	4LU	O3'-C3'-C4'	-2.84	101.95	108.81
4	H	503	4LU	C1'-N10-C10	2.79	120.91	118.41
4	D	503	4LU	C1'-N10-C10	2.72	120.84	118.41
4	D	503	4LU	C4'-C3'-C2'	-2.67	107.80	113.36
4	D	503	4LU	O1P-P-O2P	2.55	120.67	110.68
4	D	503	4LU	C1'-N10-C9A	2.55	120.30	118.29
4	D	503	4LU	C8M-C8-C9	-2.38	114.64	120.34
4	M	504	4LU	C8M-C8-C9	-2.36	114.70	120.34
4	H	503	4LU	O3'-C3'-C2'	2.32	114.41	108.81
4	M	504	4LU	C4A-C4-N3	-2.31	120.28	123.43
4	D	503	4LU	C5A-C9A-N10	-2.20	118.67	120.43
4	H	503	4LU	O1P-P-O3P	2.14	115.82	107.64
4	D	503	4LU	C9-C8-C7	2.14	122.04	119.87
4	M	504	4LU	C8M-C8-C7	2.08	124.41	121.17
4	A	503	4LU	C7-C6-C5A	-2.06	117.01	119.06
4	A	503	4LU	C4A-C10-N10	2.05	122.41	120.30
4	H	503	4LU	C9-C8-C7	2.04	121.94	119.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	A	503	4LU	C4'-C5'-O5'-P
4	H	503	4LU	C2'-C3'-C4'-C5'
4	D	503	4LU	C4'-C5'-O5'-P
4	M	504	4LU	C4'-C5'-O5'-P
4	H	503	4LU	C4'-C5'-O5'-P
4	A	503	4LU	O3'-C3'-C4'-C5'

There are no ring outliers.

8 monomers are involved in 29 short contacts:

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

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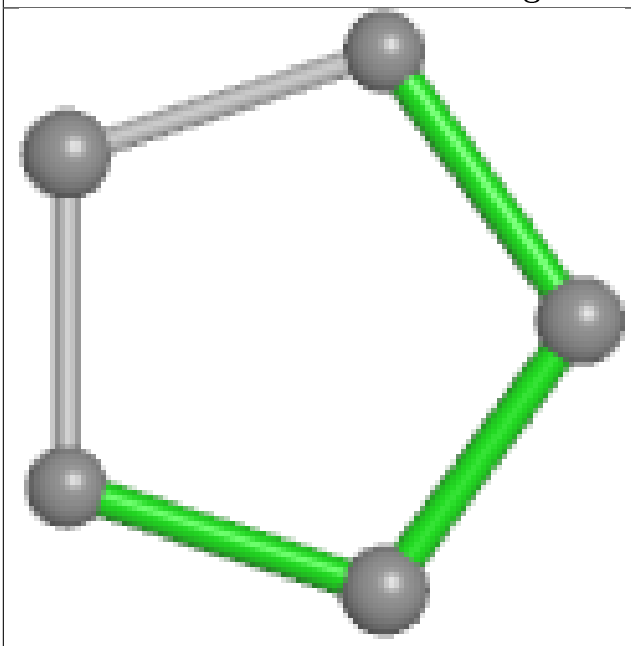
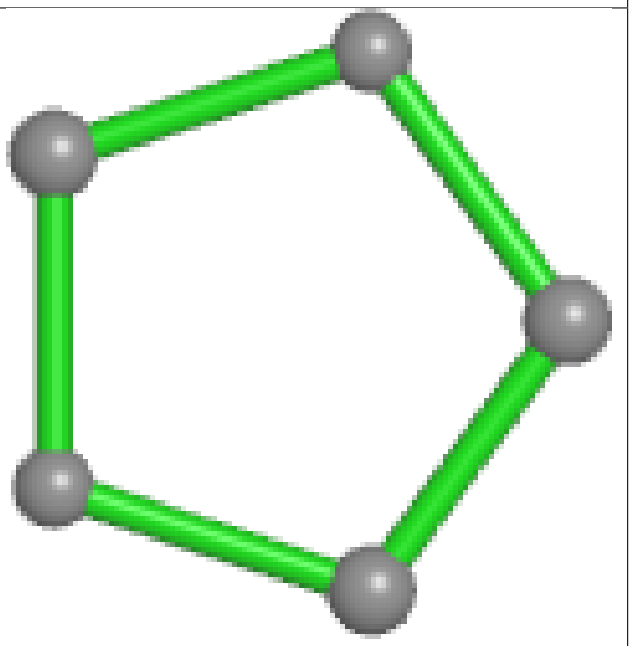
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	4LU	8	0
4	M	504	4LU	2	0
5	H	504	IMD	2	0

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 then 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.

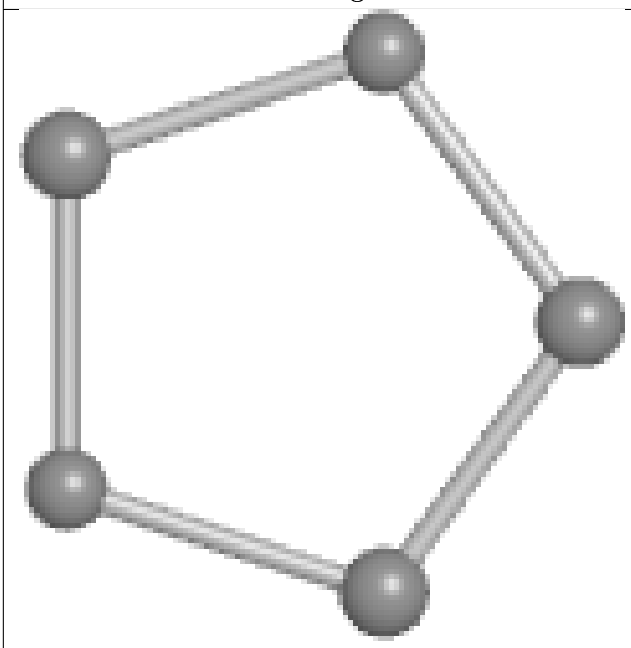
Ligand IMD A 504



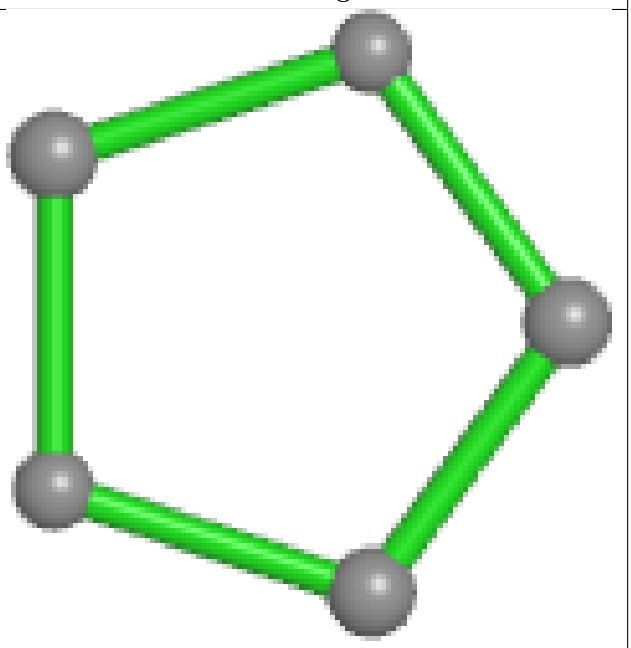
Bond lengths



Bond angles

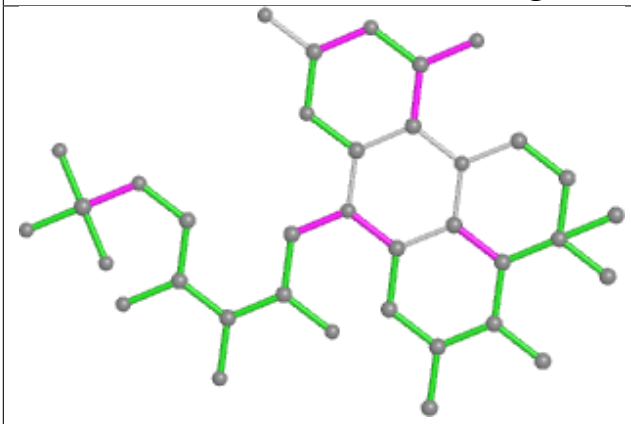


Torsions

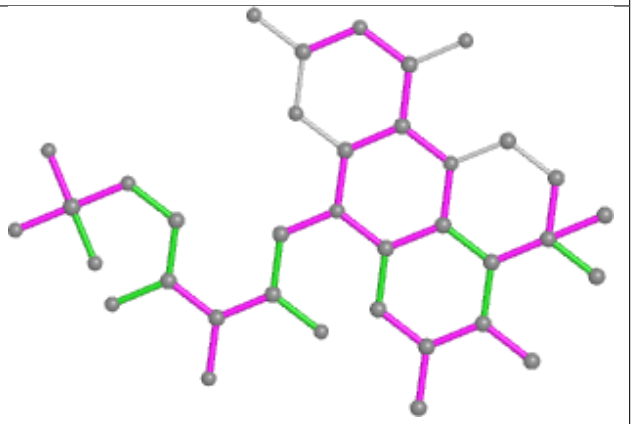


Rings

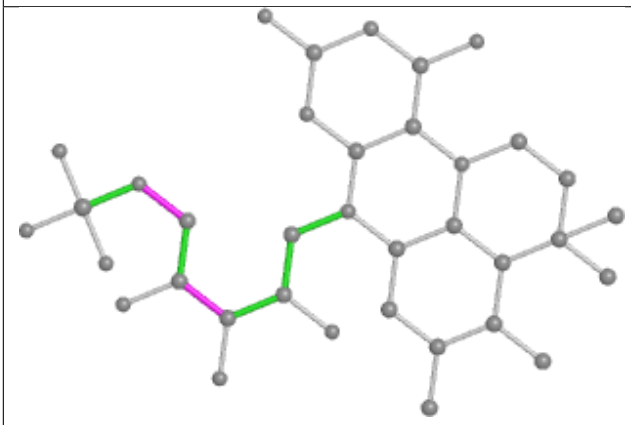
Ligand 4LU H 503



Bond lengths



Bond angles



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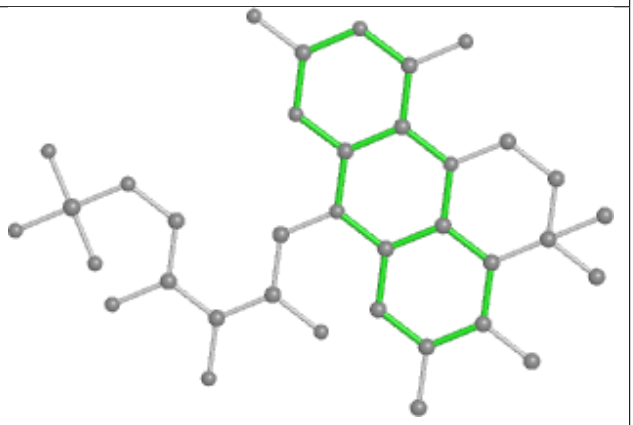
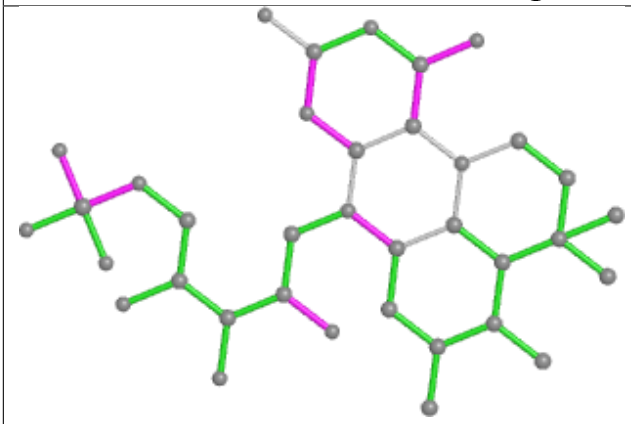
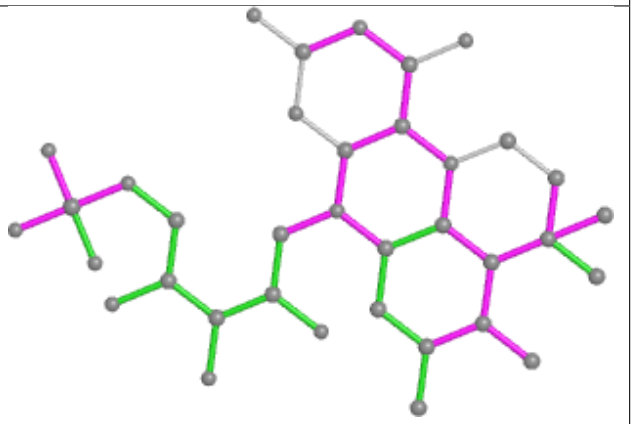


Rings

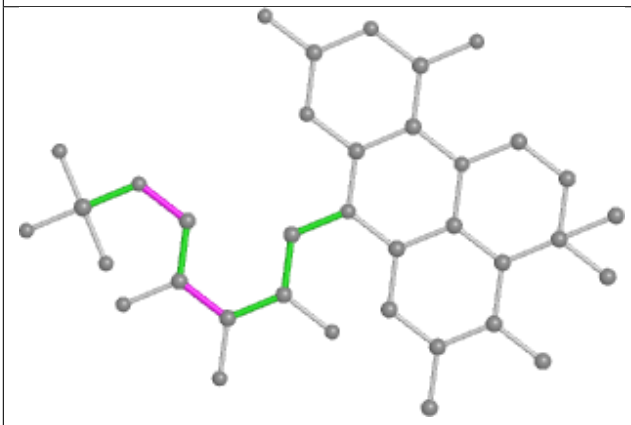
Ligand 4LU A 503



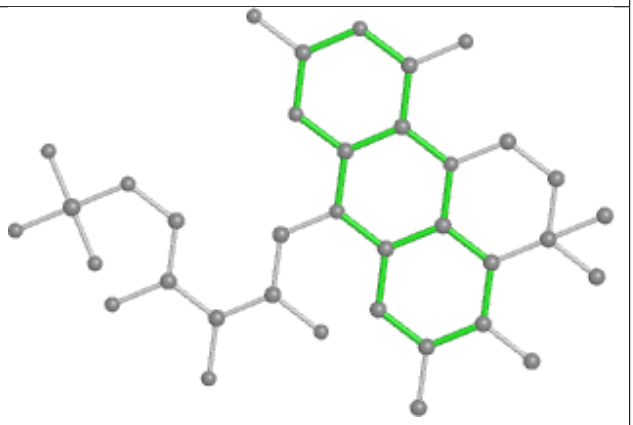
Bond lengths



Bond angles

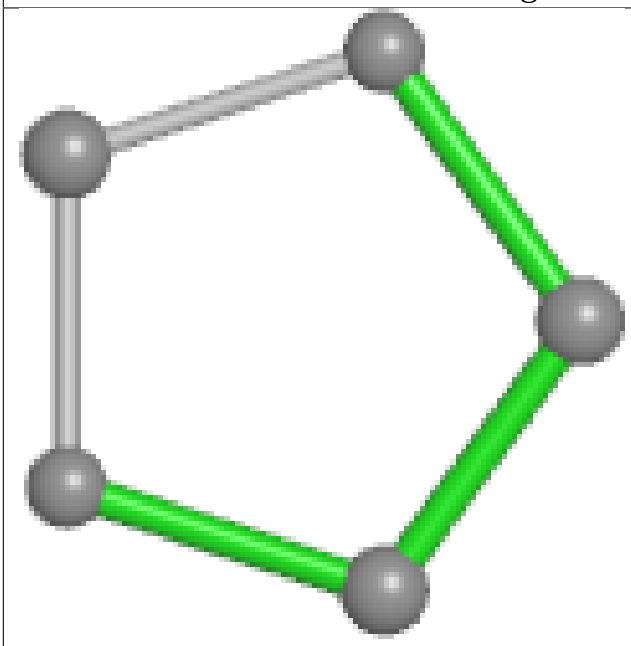


Torsions

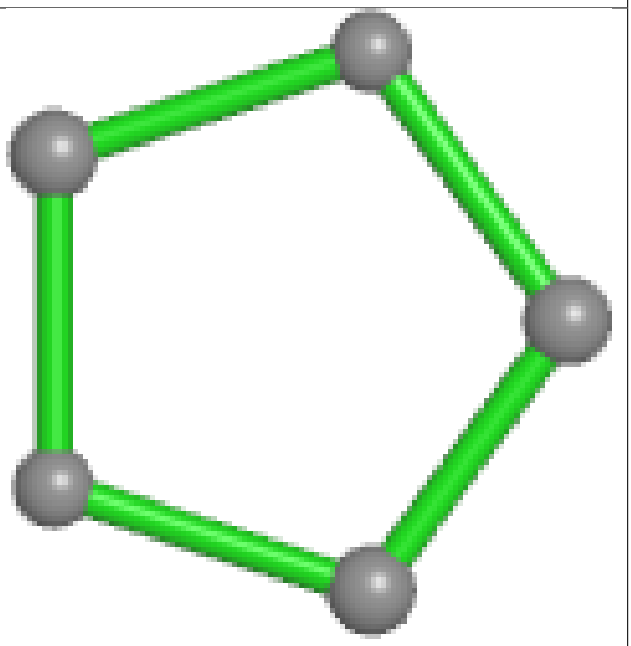


Rings

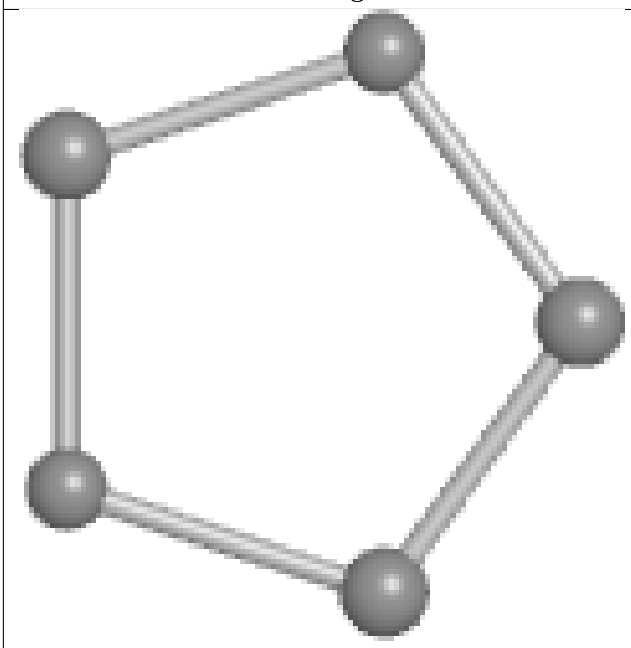
Ligand IMD M 501



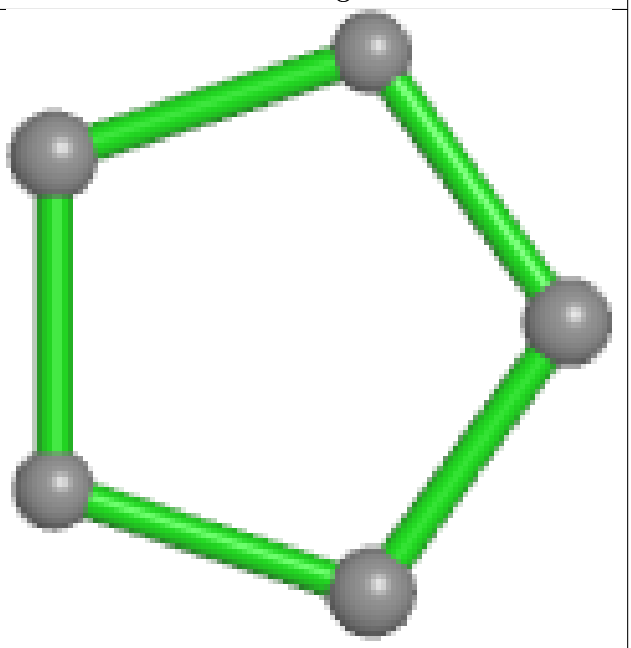
Bond lengths



Bond angles

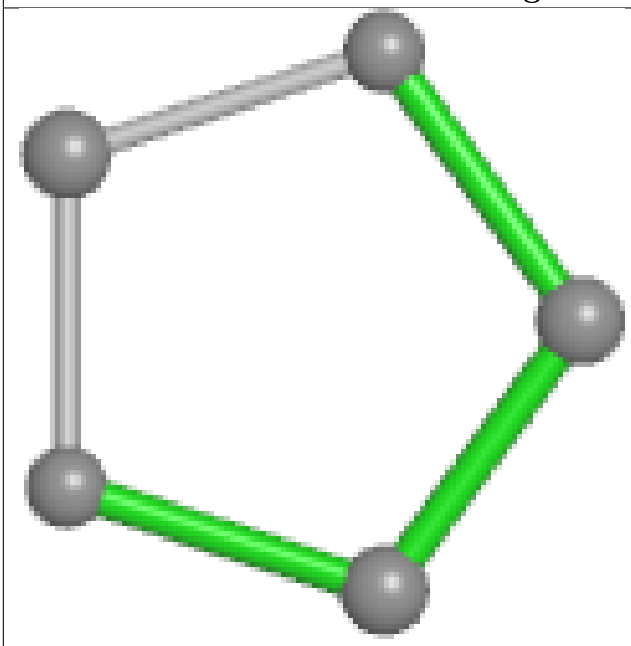


Torsions

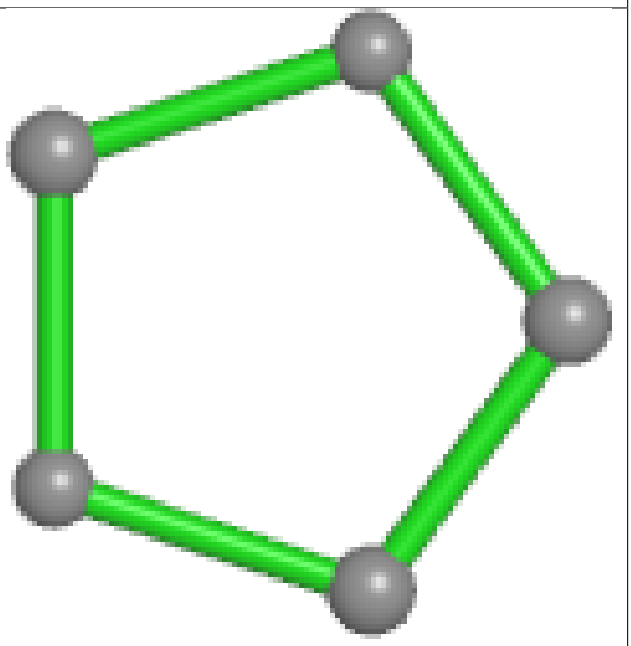


Rings

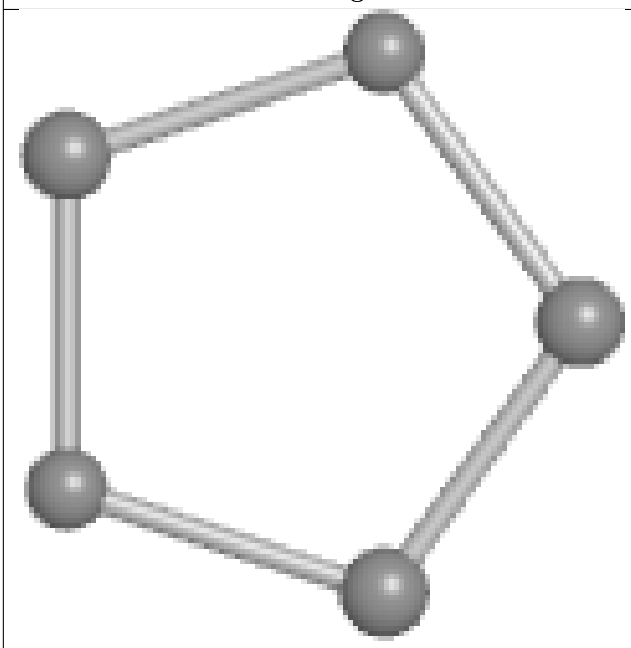
Ligand IMD D 504



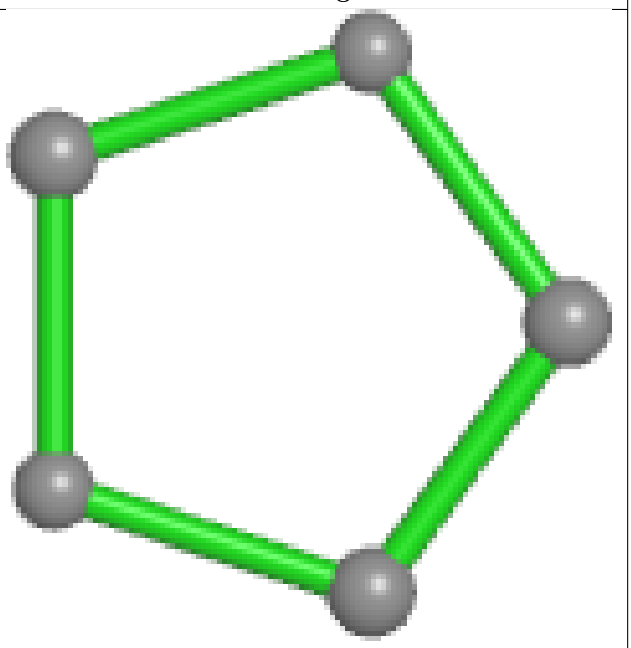
Bond lengths



Bond angles

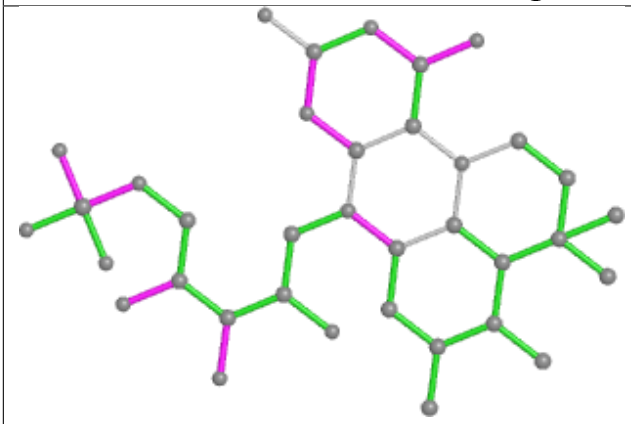


Torsions

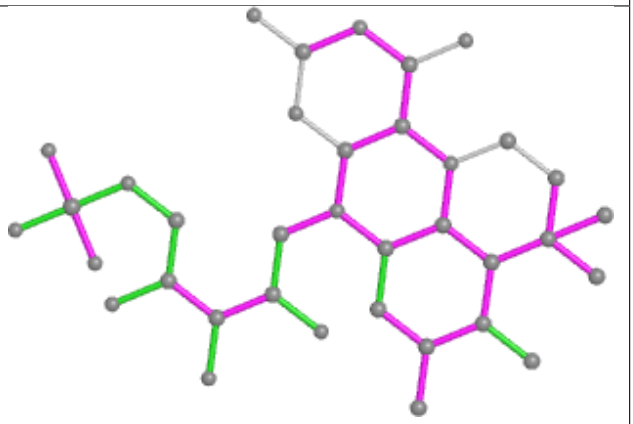


Rings

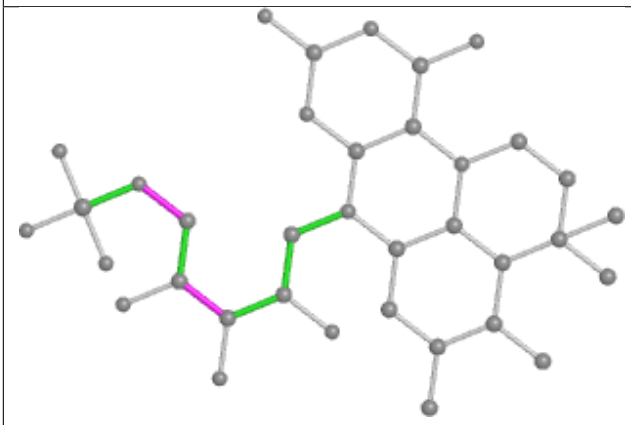
Ligand 4LU D 503



Bond lengths



Bond angles



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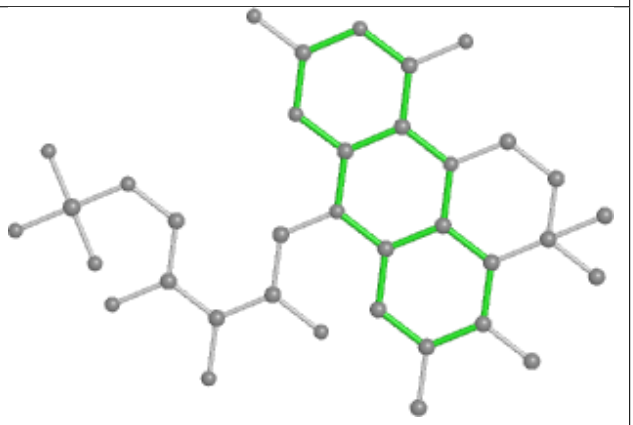
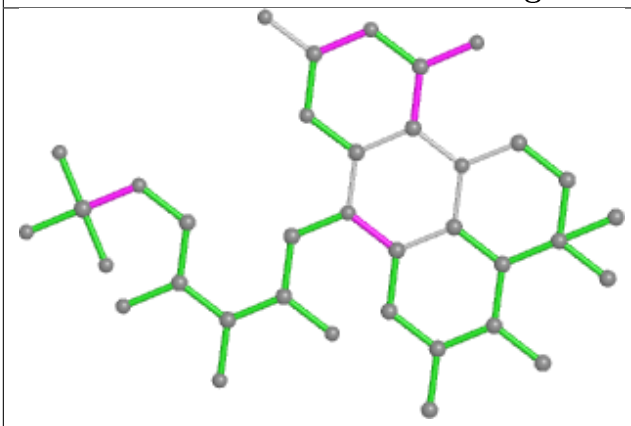
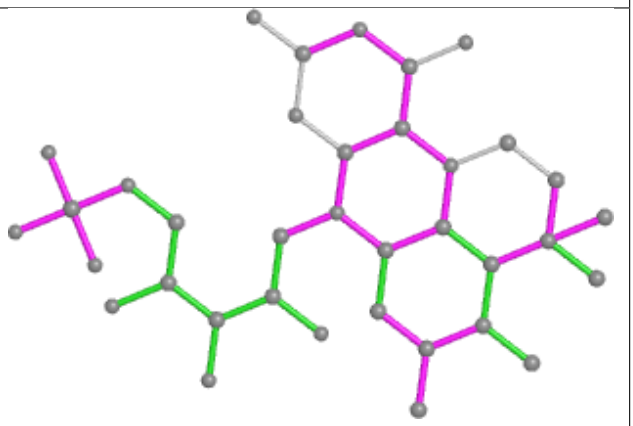


Rings

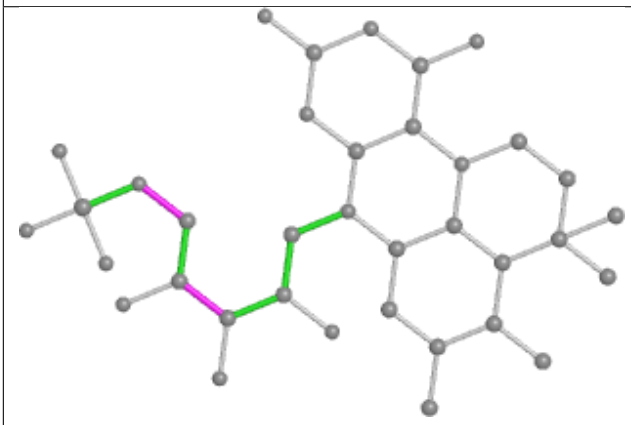
Ligand 4LU M 504



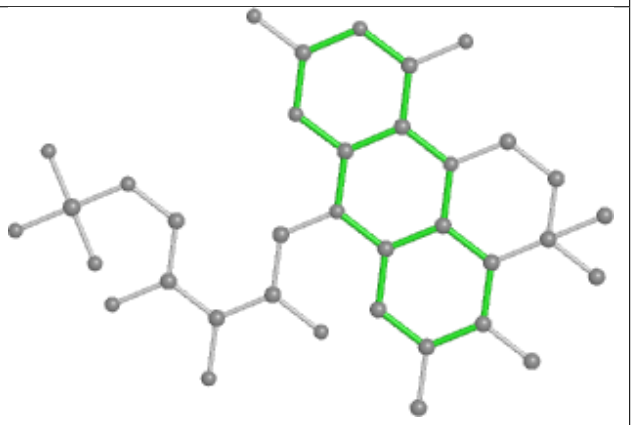
Bond lengths



Bond angles

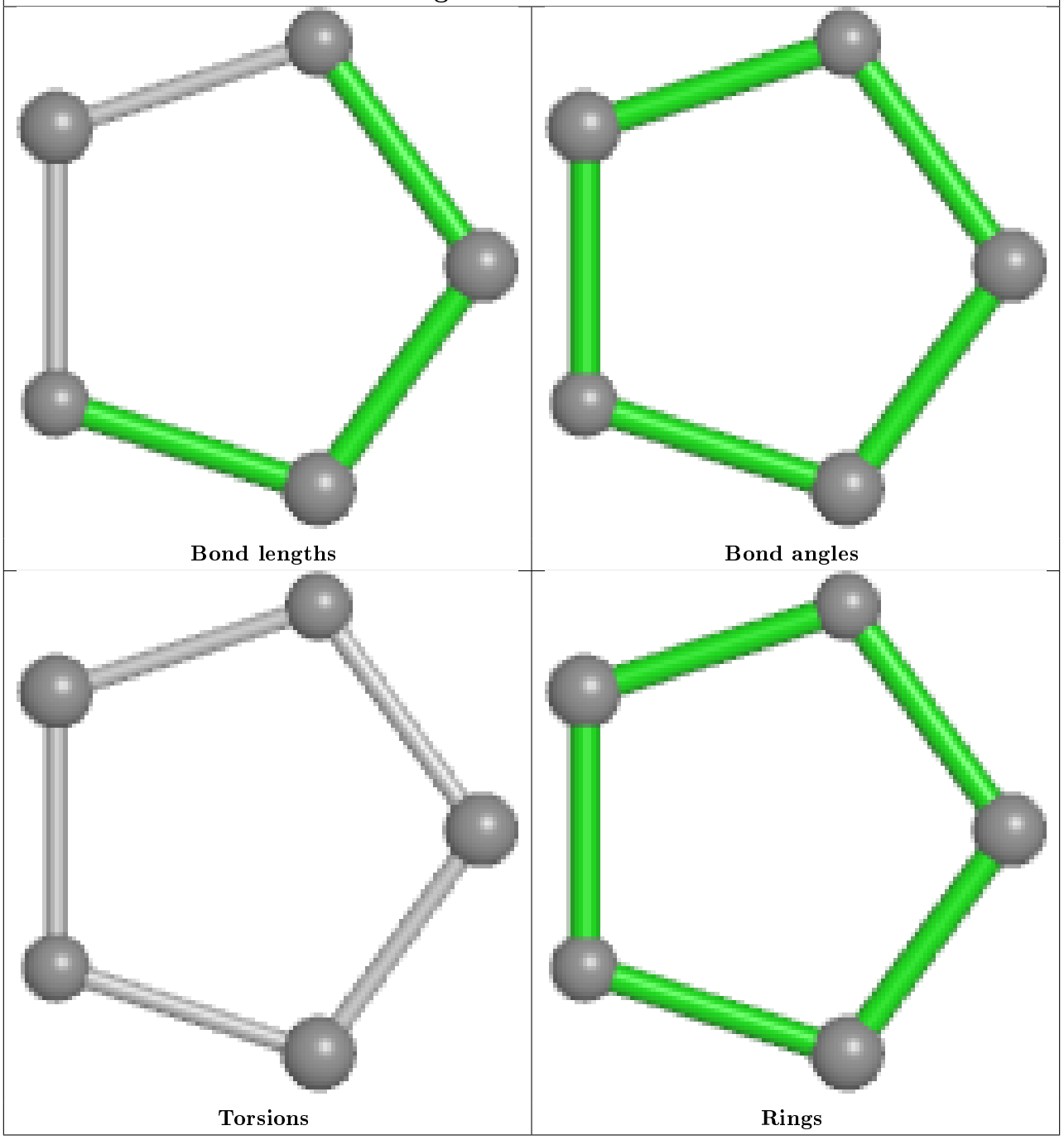


Torsions



Rings

Ligand IMD H 504



5.7 Other polymers

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, 95^{th} 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%)	-0.26	0	100	100	8, 16, 33, 51	0
1	D	496/496 (100%)	-0.26	1 (0%)	95	95	9, 16, 32, 53	0
1	H	494/496 (99%)	-0.19	1 (0%)	95	95	9, 17, 34, 46	0
1	M	494/496 (99%)	-0.21	4 (0%)	86	88	9, 17, 33, 53	0
All	All	1980/1984 (99%)	-0.23	6 (0%)	94	94	8, 17, 33, 53	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	198	ARG	3.2
1	H	199	LEU	3.2
1	M	116	ARG	2.2
1	D	1	MET	2.2
1	M	158	THR	2.2
1	M	494	GLY	2.1

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 monosaccharides 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,

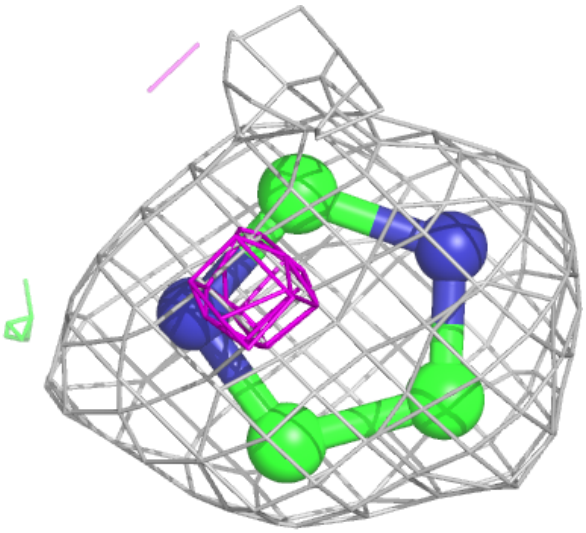
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

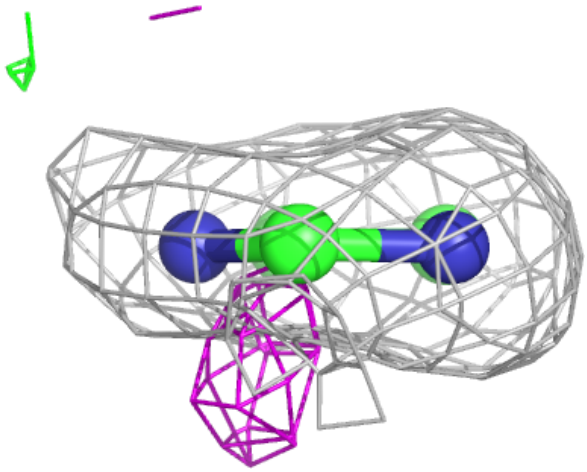
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IMD	D	504	5/5	0.92	0.10	20,22,23,23	0
5	IMD	H	504	5/5	0.92	0.16	19,20,21,22	0
5	IMD	A	504	5/5	0.94	0.17	23,25,27,28	0
5	IMD	M	501	5/5	0.94	0.09	17,19,20,20	0
4	4LU	M	504	36/36	0.95	0.09	12,15,20,20	0
4	4LU	H	503	36/36	0.96	0.08	10,15,20,22	0
4	4LU	D	503	36/36	0.96	0.09	10,14,19,20	0
4	4LU	A	503	36/36	0.96	0.09	10,14,19,21	0
2	MN	A	501	1/1	0.99	0.06	15,15,15,15	0
3	K	A	502	1/1	0.99	0.07	15,15,15,15	0
3	K	D	502	1/1	1.00	0.05	15,15,15,15	0
2	MN	D	501	1/1	1.00	0.06	14,14,14,14	0
3	K	H	502	1/1	1.00	0.05	16,16,16,16	0
3	K	M	503	1/1	1.00	0.05	15,15,15,15	0
2	MN	H	501	1/1	1.00	0.04	14,14,14,14	0
2	MN	M	502	1/1	1.00	0.04	15,15,15,15	0

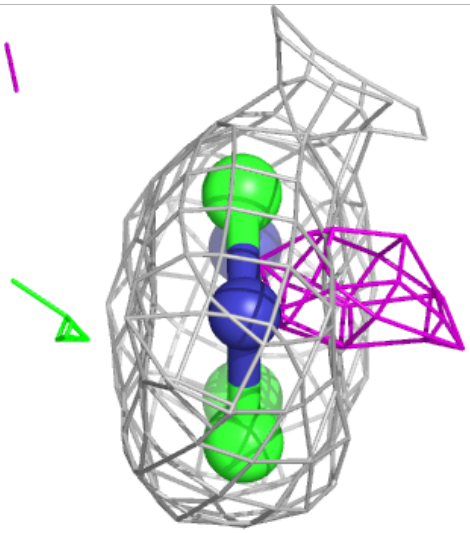
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IMD 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)

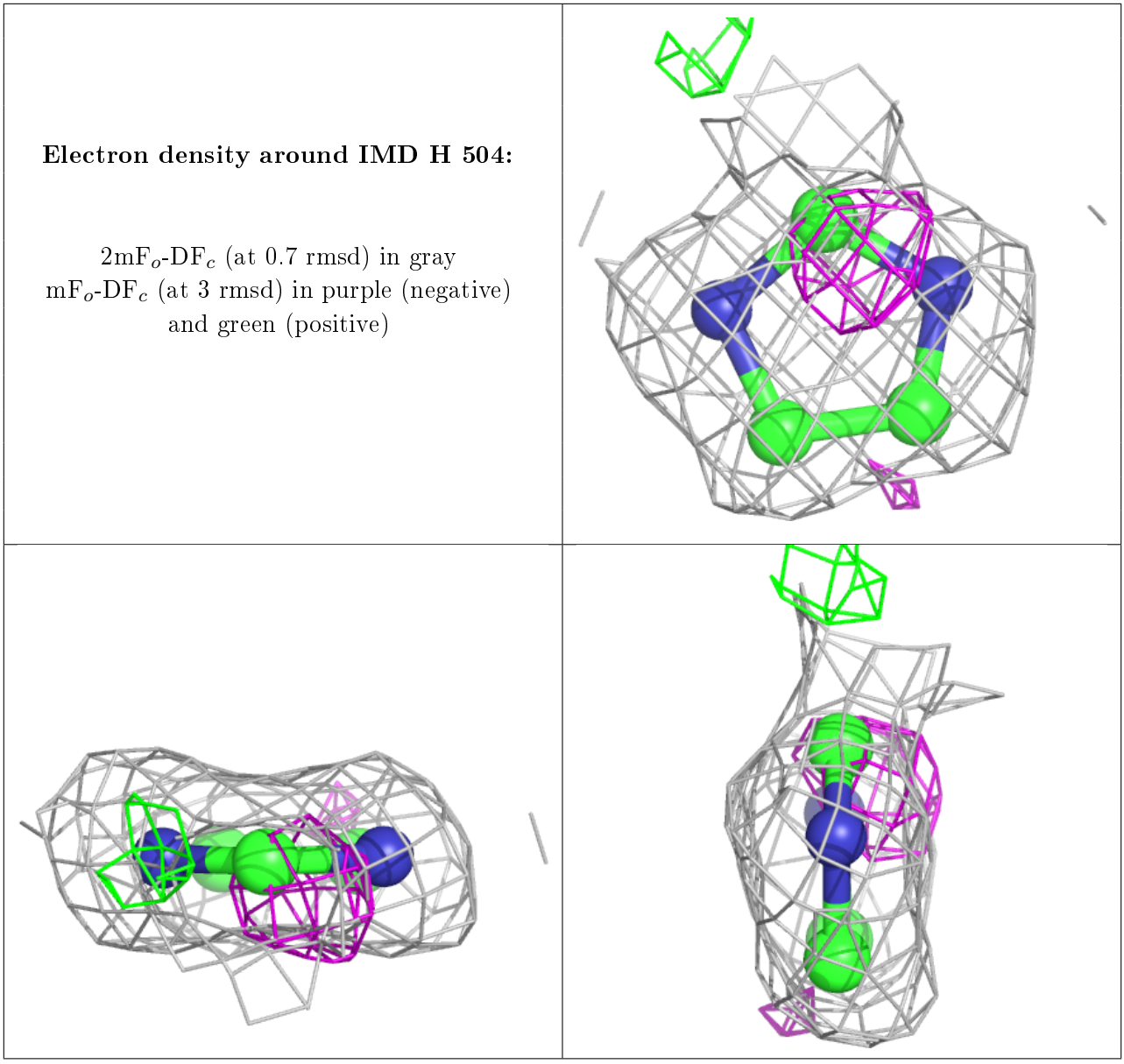






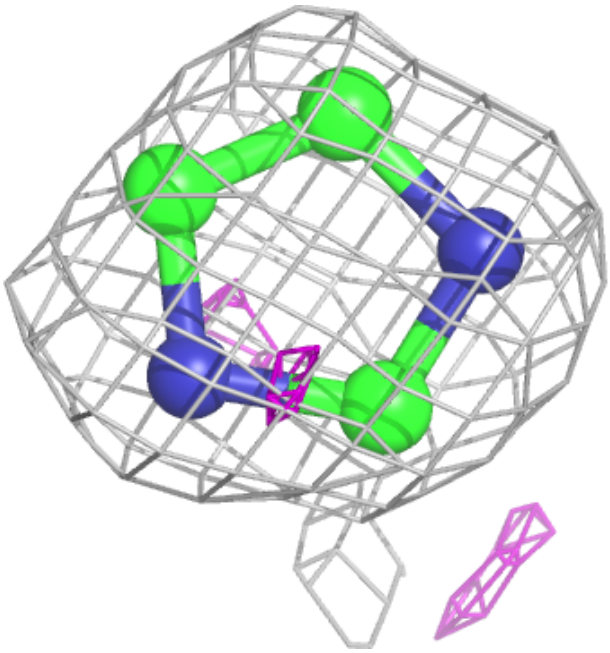
Electron density around IMD H 504:

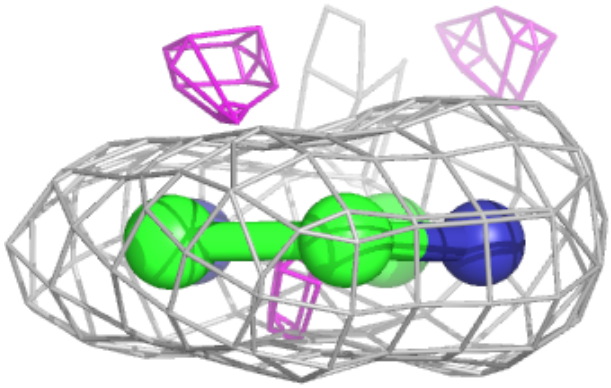
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

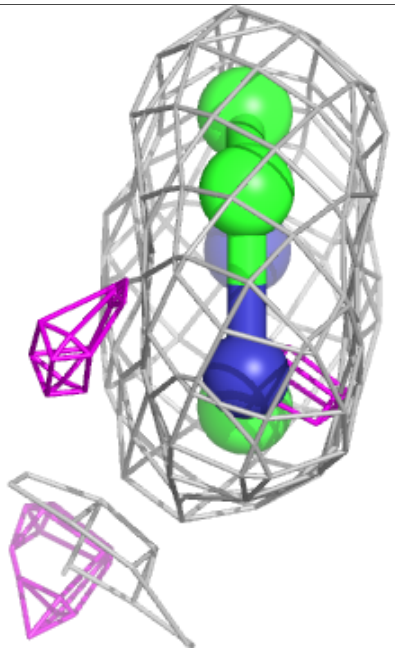


Electron density around IMD A 504:

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

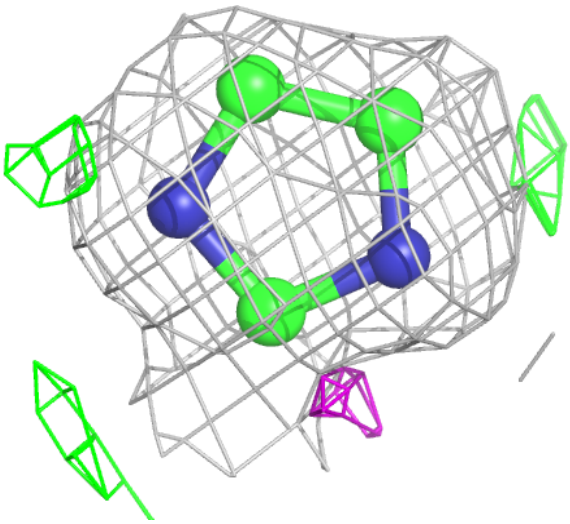


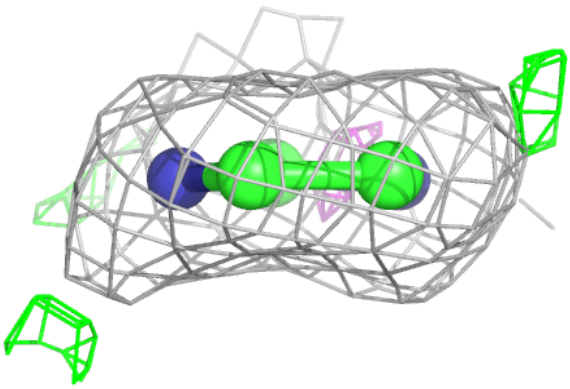


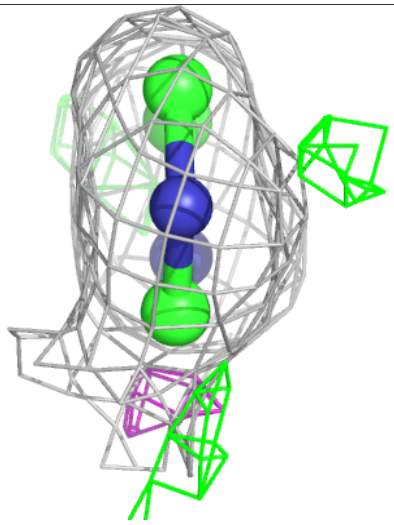


Electron density around IMD M 501:

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

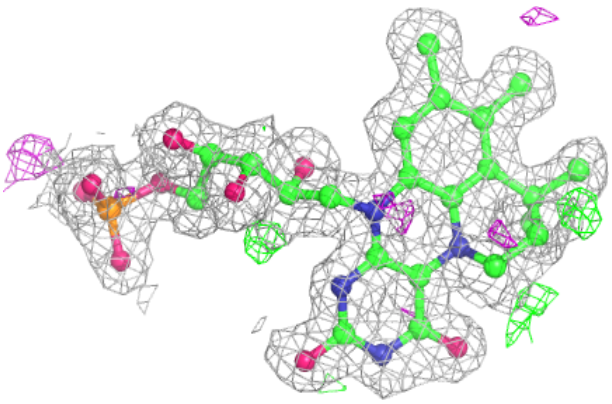


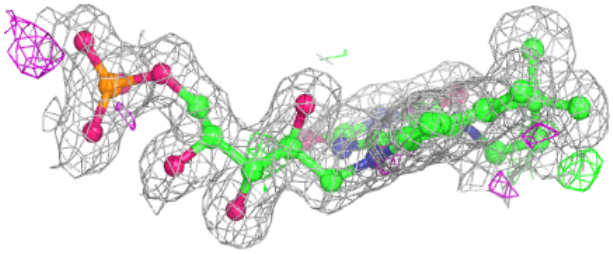




Electron density around 4LU M 504:

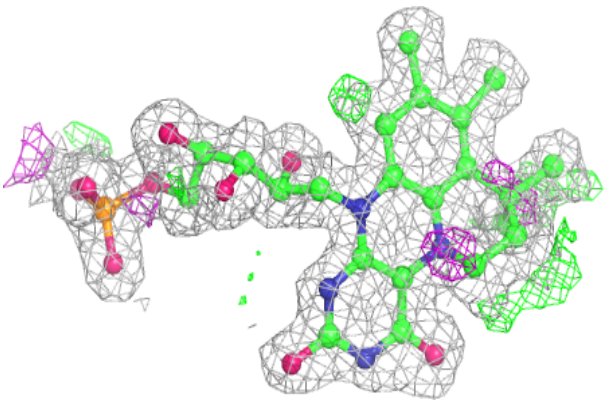
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

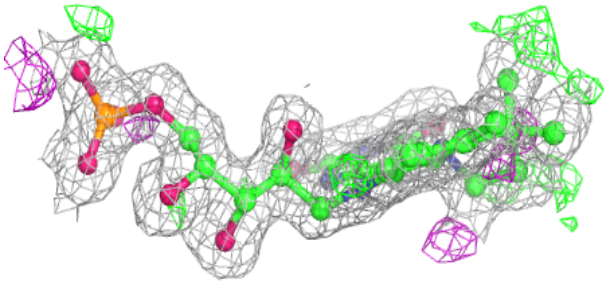


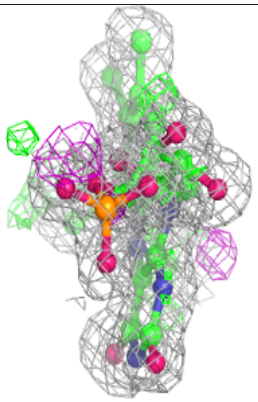


Electron density around 4LU H 503:

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

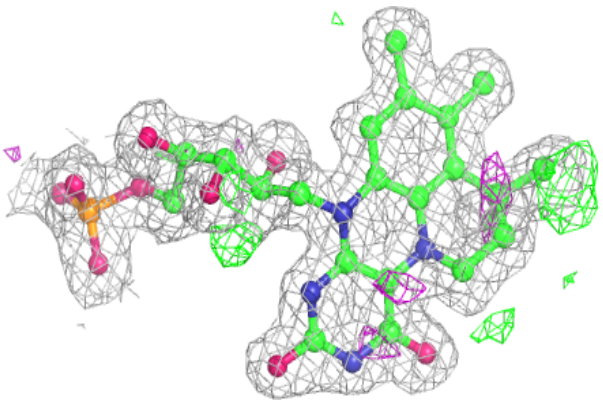


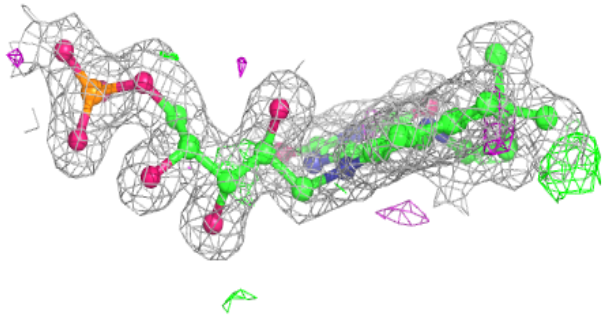


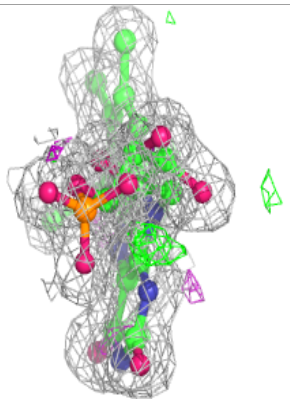


Electron density around 4LU D 503:

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

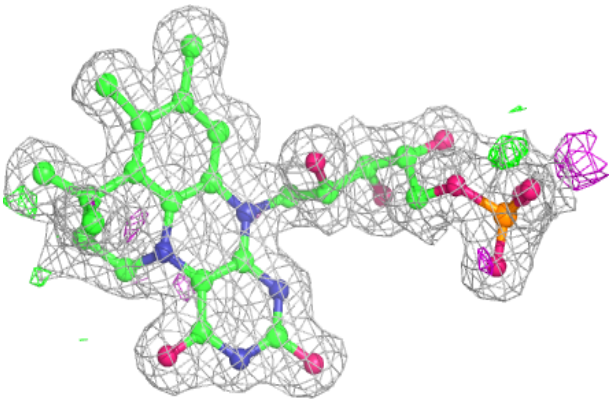


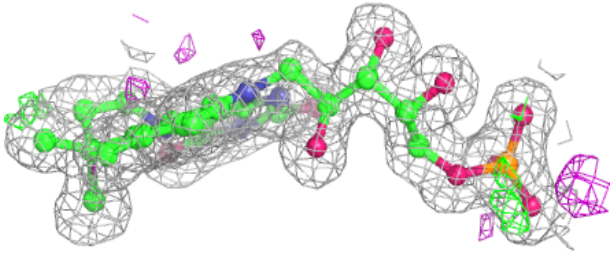


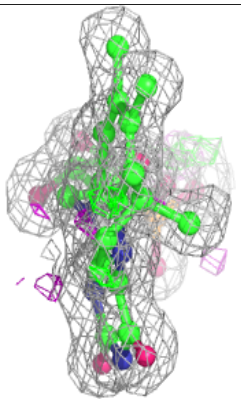


Electron density around 4LU A 503:

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







6.5 Other polymers (i)

There are no such residues in this entry.