



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2022 – 04:49 pm BST

PDB ID : 8A0U  
Title : Crystal structure of TEAD3 in complex with CPD4  
Authors : Scheufler, C.; Kallen, J.  
Deposited on : 2022-05-30  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

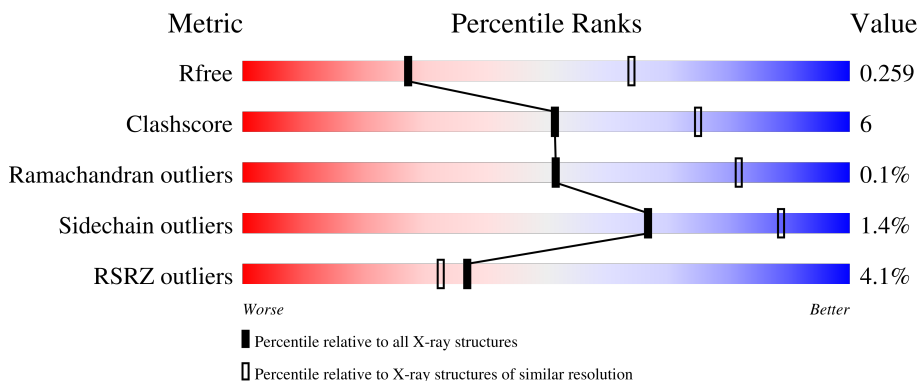
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	222	 4% 82% 13% 6%
1	B	222	 3% 82% 12% 6%
1	C	222	 5% 79% 14% 7%
1	D	222	 4% 82% 12% 6%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7122 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 Transcriptional enhancer factor TEF-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	1665	1075	277	305	8	0	1	0
1	B	209	1696	1089	284	315	8	0	2	0
1	C	206	1664	1071	278	307	8	0	1	0
1	D	208	1663	1071	275	309	8	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

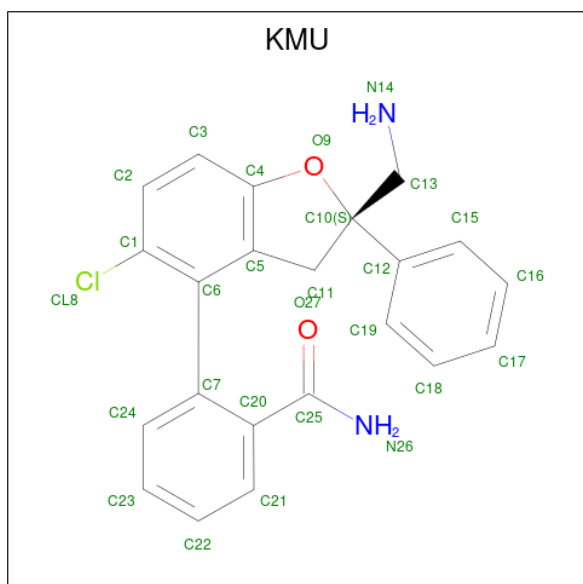
Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	expression tag	UNP P70210
A	216	PRO	-	expression tag	UNP P70210
A	217	GLY	-	expression tag	UNP P70210
A	436	GLY	-	expression tag	UNP P70210
B	215	GLY	-	expression tag	UNP P70210
B	216	PRO	-	expression tag	UNP P70210
B	217	GLY	-	expression tag	UNP P70210
B	436	GLY	-	expression tag	UNP P70210
C	215	GLY	-	expression tag	UNP P70210
C	216	PRO	-	expression tag	UNP P70210
C	217	GLY	-	expression tag	UNP P70210
C	436	GLY	-	expression tag	UNP P70210
D	215	GLY	-	expression tag	UNP P70210
D	216	PRO	-	expression tag	UNP P70210
D	217	GLY	-	expression tag	UNP P70210
D	436	GLY	-	expression tag	UNP P70210

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



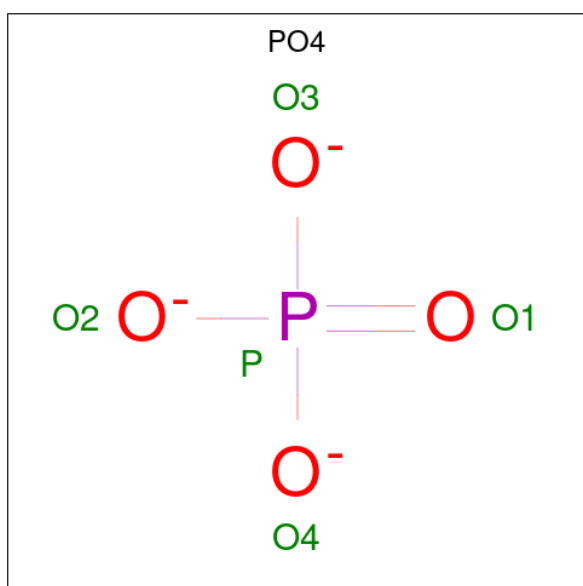
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			15	14 1		
2	B	1	Total	C O	0	0
			15	14 1		
2	C	1	Total	C O	0	0
			15	14 1		
2	D	1	Total	C O	0	0
			15	14 1		

- Molecule 3 is 2-[(2 {S})-2-(aminomethyl)-5-chloranyl-2-phenyl-3 {H}-1-benzofuran-4-yl]benzamide (three-letter code: KMU) (formula:  $C_{22}H_{19}ClN_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	0	0
			27	22	1	2	2		
3	B	1	Total	C	Cl	N	O	0	0
			27	22	1	2	2		
3	C	1	Total	C	Cl	N	O	0	0
			27	22	1	2	2		
3	D	1	Total	C	Cl	N	O	0	0
			27	22	1	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

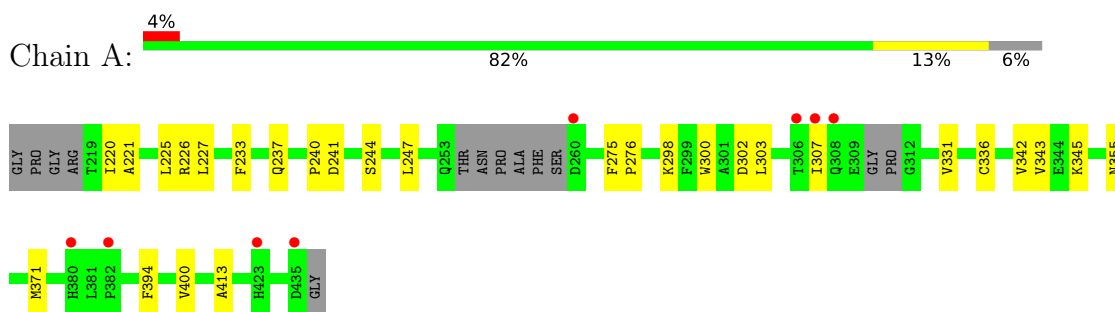
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	59	Total O 59 59	0	0
5	C	57	Total O 57 57	0	0
5	D	55	Total O 55 55	0	0

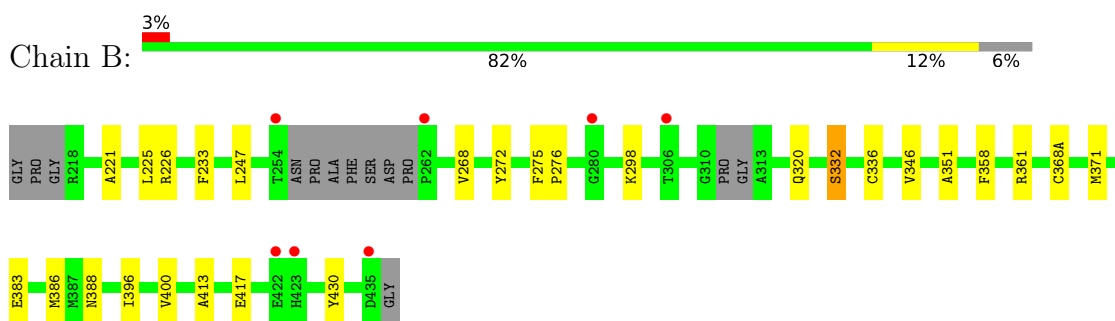
### 3 Residue-property plots [i](#)

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.

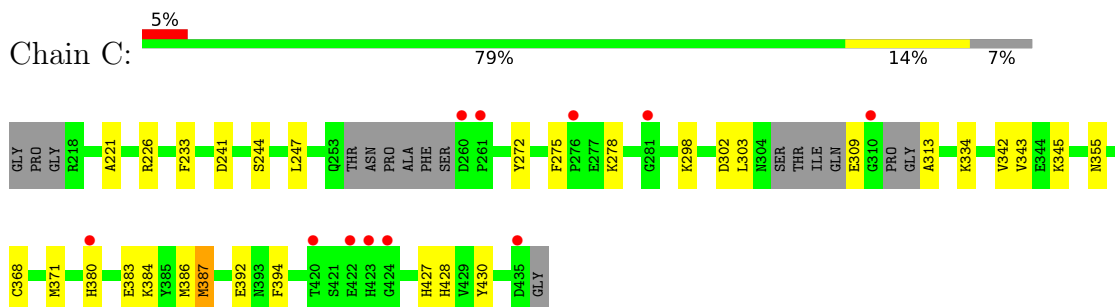
- Molecule 1: Transcriptional enhancer factor TEF-5



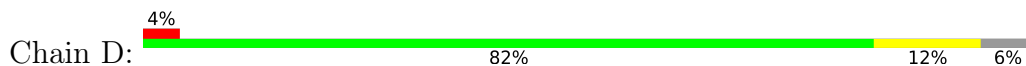
- Molecule 1: Transcriptional enhancer factor TEF-5

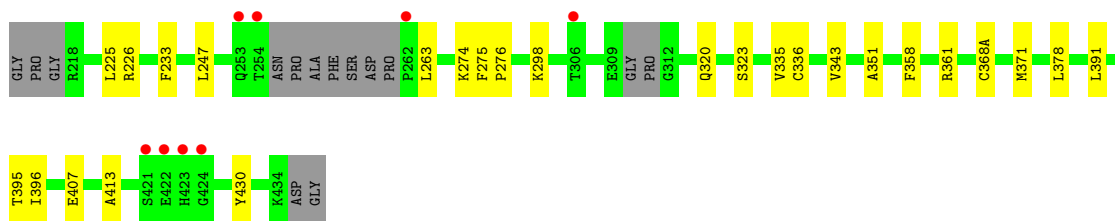


- Molecule 1: Transcriptional enhancer factor TEF-5



- Molecule 1: Transcriptional enhancer factor TEF-5







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.27Å 128.61Å 156.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.64 – 2.90 24.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (24.64-2.90) 92.5 (24.64-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.89Å)	Xtriage
Refinement program	BUSTER 2.11.8 (3-FEB-2022)	Depositor
R, $R_{free}$	0.212 , 0.268 0.209 , 0.259	Depositor DCC
$R_{free}$ test set	1383 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MYR, KMU, PO4

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	0.43	0/1704	0.61	0/2304
1	B	0.43	0/1735	0.63	0/2342
1	C	0.44	0/1702	0.62	0/2297
1	D	0.43	0/1700	0.61	0/2295
All	All	0.43	0/6841	0.62	0/9238

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1665	0	1616	17	0
1	B	1696	0	1652	21	0
1	C	1664	0	1617	20	0
1	D	1663	0	1616	20	0
2	A	15	0	27	3	0
2	B	15	0	27	8	0
2	C	15	0	27	3	0
2	D	15	0	27	8	0
3	A	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	0	0
3	C	27	0	0	1	0
3	D	27	0	0	1	0
4	A	15	0	0	0	0
4	C	15	0	0	0	0
4	D	10	0	0	0	0
5	A	55	0	0	0	0
5	B	59	0	0	0	0
5	C	57	0	0	2	0
5	D	55	0	0	0	0
All	All	7122	0	6609	76	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 6.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:MET:HG3	2:D:501:MYR:H51	1.60	0.81
1:B:371:MET:HG3	2:B:501:MYR:H51	1.65	0.78
1:C:221:ALA:HB2	1:C:226:ARG:HG3	1.69	0.74
1:B:221:ALA:HB2	1:B:226:ARG:HG3	1.70	0.72
1:A:221:ALA:HB2	1:A:226:ARG:HG3	1.74	0.70
1:B:351:ALA:HB3	1:C:355:ASN:HB3	1.76	0.67
1:C:371:MET:HG3	2:C:501:MYR:H31	1.77	0.66
1:D:371:MET:HG3	2:D:501:MYR:H21	1.77	0.66
1:A:371:MET:HG3	2:A:501:MYR:H31	1.77	0.66
1:A:355:ASN:HB3	1:D:351:ALA:HB3	1.77	0.65
1:D:368(A):CYS:H	2:D:501:MYR:H22	1.62	0.65
1:C:342:VAL:HG23	1:C:343:VAL:HG23	1.80	0.63
1:B:371:MET:HG3	2:B:501:MYR:H21	1.81	0.63
1:D:378:LEU:HD11	1:D:391:LEU:HD21	1.82	0.62
1:B:368(A):CYS:H	2:B:501:MYR:H22	1.64	0.60
1:B:368(A):CYS:H	2:B:501:MYR:C1	2.17	0.58
1:D:368(A):CYS:H	2:D:501:MYR:C1	2.17	0.57
1:B:276:PRO:HD3	1:B:336:CYS:SG	2.45	0.57
1:A:241:ASP:OD2	1:C:302:ASP:OD2	2.23	0.57
1:A:342:VAL:HG23	1:A:343:VAL:HG23	1.86	0.56
1:D:320:GLN:HG3	1:D:361:ARG:HG2	1.86	0.56
1:C:394:PHE:CE2	2:C:501:MYR:H141	2.41	0.55
1:C:384:LYS:HA	1:C:387:MET:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:MET:CG	2:D:501:MYR:H21	2.37	0.54
1:C:303:LEU:HD21	2:C:501:MYR:H112	1.88	0.54
1:D:233:PHE:HB3	1:D:247:LEU:HD23	1.88	0.54
1:C:233:PHE:HB3	1:C:247:LEU:HD23	1.89	0.54
1:C:428:HIS:ND1	1:C:430:TYR:CZ	2.76	0.54
1:D:368(A):CYS:H	2:D:501:MYR:C2	2.21	0.54
1:B:371:MET:CG	2:B:501:MYR:H21	2.38	0.53
1:B:368(A):CYS:H	2:B:501:MYR:C2	2.23	0.52
1:A:233:PHE:HB3	1:A:247:LEU:HD23	1.90	0.52
1:A:331:VAL:HG22	1:A:400:VAL:HG22	1.91	0.52
1:B:332:SER:HB2	1:B:346:VAL:HG22	1.92	0.51
1:A:303:LEU:HD21	2:A:501:MYR:H112	1.95	0.49
1:D:275:PHE:CZ	1:D:413:ALA:HB1	2.48	0.49
1:A:220:ILE:HD13	1:A:227:LEU:HD23	1.95	0.49
1:A:394:PHE:CE2	2:A:501:MYR:H141	2.48	0.48
1:A:302:ASP:OD2	1:C:241:ASP:OD2	2.32	0.47
1:C:392:GLU:OE1	3:C:502:KMU:N14	2.47	0.47
2:D:501:MYR:H121	2:D:501:MYR:H92	1.56	0.47
1:B:233:PHE:HB3	1:B:247:LEU:HD23	1.95	0.47
1:C:298:LYS:HD2	1:C:430:TYR:CE2	2.50	0.47
1:C:298:LYS:HD2	1:C:430:TYR:HE2	1.78	0.47
1:D:351:ALA:HB1	1:D:358:PHE:HB3	1.96	0.46
1:B:396:ILE:HD13	2:B:501:MYR:H62	1.98	0.45
1:C:383:GLU:HB2	1:C:386:MET:HG3	1.98	0.45
1:D:298:LYS:HD2	1:D:430:TYR:HE2	1.80	0.45
1:C:380:HIS:HE1	5:C:652:HOH:O	1.98	0.45
1:D:335:VAL:HG22	1:D:396:ILE:HG12	1.99	0.45
1:A:298:LYS:HE2	1:A:300:TRP:CH2	2.52	0.44
1:D:298:LYS:HD2	1:D:430:TYR:CE2	2.52	0.44
1:D:276:PRO:HD3	1:D:336:CYS:SG	2.56	0.44
2:B:501:MYR:H111	2:B:501:MYR:H82	1.78	0.44
1:B:298:LYS:HD2	1:B:430:TYR:HE2	1.82	0.44
1:C:309:GLU:HG3	1:C:313:ALA:CB	2.47	0.43
1:B:268:VAL:HG22	1:B:272:TYR:CE1	2.53	0.43
1:C:343:VAL:HG11	1:C:368:CYS:SG	2.59	0.43
1:A:237:GLN:HE21	1:A:240:PRO:HA	1.84	0.43
1:B:320:GLN:HG2	1:B:361:ARG:HG2	2.01	0.43
1:A:276:PRO:HD3	1:A:336:CYS:SG	2.58	0.42
1:B:388:ASN:OD1	1:B:417:GLU:HG2	2.20	0.42
1:B:351:ALA:HB1	1:B:358:PHE:HB3	2.02	0.42
1:D:274:LYS:HD2	3:D:502:KMU:CL8	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:TYR:O	1:C:275:PHE:O	2.37	0.41
1:D:396:ILE:HD13	2:D:501:MYR:H62	2.01	0.41
1:B:298:LYS:HD2	1:B:430:TYR:CE2	2.54	0.41
1:D:275:PHE:CZ	1:D:395:THR:HB	2.56	0.41
1:A:244:SER:HB3	1:A:307:ILE:HG21	2.02	0.41
1:B:383:GLU:HB2	1:B:386:MET:HG3	2.02	0.41
1:A:275:PHE:CZ	1:A:413:ALA:HB1	2.56	0.41
1:B:275:PHE:CZ	1:B:413:ALA:HB1	2.56	0.41
1:C:427:HIS:HD2	5:C:637:HOH:O	2.03	0.41
1:A:225:LEU:HD22	1:A:400:VAL:HG11	2.04	0.40
1:B:225:LEU:HD22	1:B:400:VAL:HG11	2.04	0.40
1:D:225:LEU:HD12	1:D:323:SER:HB3	2.04	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	204/222 (92%)	200 (98%)	4 (2%)	0	100	100
1	B	205/222 (92%)	201 (98%)	4 (2%)	0	100	100
1	C	199/222 (90%)	197 (99%)	1 (0%)	1 (0%)	29	61
1	D	203/222 (91%)	197 (97%)	6 (3%)	0	100	100
All	All	811/888 (91%)	795 (98%)	15 (2%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	LYS

### 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	180/198 (91%)	179 (99%)	1 (1%)	86	96
1	B	187/198 (94%)	186 (100%)	1 (0%)	88	96
1	C	182/198 (92%)	178 (98%)	4 (2%)	52	81
1	D	181/198 (91%)	177 (98%)	4 (2%)	52	81
All	All	730/792 (92%)	720 (99%)	10 (1%)	67	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	LYS
1	B	332	SER
1	C	244	SER
1	C	334	LYS
1	C	345	LYS
1	C	387	MET
1	D	226	ARG
1	D	263	LEU
1	D	343	VAL
1	D	407	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	253	GLN
1	A	427	HIS
1	B	428	HIS
1	C	380	HIS
1	C	398	GLN
1	C	427	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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	KMU	B	502	-	29,30,30	1.05	2 (6%)	33,44,44	1.42	5 (15%)
4	PO4	C	504	-	4,4,4	0.33	0	6,6,6	0.50	0
3	KMU	C	502	-	29,30,30	0.87	1 (3%)	33,44,44	1.41	4 (12%)
3	KMU	D	502	-	29,30,30	0.89	1 (3%)	33,44,44	1.34	4 (12%)
4	PO4	D	503	-	4,4,4	0.52	0	6,6,6	0.29	0
4	PO4	A	503	-	4,4,4	0.93	0	6,6,6	0.49	0
4	PO4	D	504	-	4,4,4	1.07	0	6,6,6	0.47	0
4	PO4	C	503	-	4,4,4	1.00	0	6,6,6	0.50	0
4	PO4	A	505	-	4,4,4	0.34	0	6,6,6	0.31	0
3	KMU	A	502	-	29,30,30	1.01	2 (6%)	33,44,44	1.33	4 (12%)
2	MYR	C	501	1	14,14,15	0.65	0	13,13,15	0.82	0
4	PO4	C	505	-	4,4,4	0.31	0	6,6,6	0.30	0
2	MYR	B	501	1	14,14,15	0.76	0	13,13,15	0.63	0
2	MYR	A	501	1	14,14,15	0.64	0	13,13,15	0.83	0
4	PO4	A	504	-	4,4,4	0.18	0	6,6,6	0.34	0
2	MYR	D	501	1	14,14,15	0.69	0	13,13,15	0.84	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
3	KMU	B	502	-	-	2/14/27/27	0/4/4/4
3	KMU	C	502	-	-	4/14/27/27	0/4/4/4
3	KMU	D	502	-	-	1/14/27/27	0/4/4/4
3	KMU	A	502	-	-	3/14/27/27	0/4/4/4
2	MYR	C	501	1	-	7/11/12/13	-
2	MYR	B	501	1	-	8/11/12/13	-
2	MYR	A	501	1	-	7/11/12/13	-
2	MYR	D	501	1	-	8/11/12/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	KMU	C20-C25	3.10	1.54	1.50
3	A	502	KMU	C11-C10	2.31	1.57	1.52
3	D	502	KMU	C20-C25	2.28	1.53	1.50
3	A	502	KMU	C10-C12	2.13	1.55	1.52
3	B	502	KMU	C25-N26	2.06	1.36	1.33
3	C	502	KMU	C11-C10	2.06	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	KMU	O9-C4-C5	4.64	116.67	113.12
3	C	502	KMU	O9-C4-C5	4.46	116.53	113.12
3	A	502	KMU	O9-C4-C5	3.86	116.07	113.12
3	A	502	KMU	C11-C5-C6	3.55	131.34	127.88
3	C	502	KMU	C11-C5-C6	3.29	131.08	127.88
3	D	502	KMU	O9-C4-C5	3.25	115.61	113.12
3	D	502	KMU	C10-C13-N14	-3.18	108.88	115.29
3	D	502	KMU	C11-C5-C6	3.12	130.91	127.88
3	B	502	KMU	C10-O9-C4	-2.95	104.16	107.38
3	B	502	KMU	C11-C5-C6	2.82	130.62	127.88
3	C	502	KMU	C10-O9-C4	-2.69	104.44	107.38
3	D	502	KMU	C24-C7-C20	2.64	121.02	118.03
3	A	502	KMU	O27-C25-C20	-2.50	117.30	120.24
3	A	502	KMU	C20-C25-N26	2.48	122.10	118.29
3	B	502	KMU	C24-C7-C20	2.19	120.52	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	KMU	C10-C13-N14	-2.14	110.98	115.29
3	B	502	KMU	O27-C25-N26	-2.13	119.55	122.58

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	MYR	C1-C2-C3-C4
2	D	501	MYR	C1-C2-C3-C4
2	B	501	MYR	C11-C10-C9-C8
2	D	501	MYR	C9-C10-C11-C12
2	A	501	MYR	C5-C6-C7-C8
2	B	501	MYR	C6-C7-C8-C9
2	B	501	MYR	C7-C8-C9-C10
2	C	501	MYR	C5-C6-C7-C8
2	D	501	MYR	C6-C7-C8-C9
2	B	501	MYR	C9-C10-C11-C12
2	B	501	MYR	C5-C6-C7-C8
2	D	501	MYR	C11-C10-C9-C8
2	D	501	MYR	C7-C8-C9-C10
2	D	501	MYR	C10-C11-C12-C13
2	A	501	MYR	C7-C8-C9-C10
2	C	501	MYR	C7-C8-C9-C10
2	A	501	MYR	C11-C12-C13-C14
2	C	501	MYR	C11-C12-C13-C14
2	B	501	MYR	C11-C12-C13-C14
2	C	501	MYR	C4-C5-C6-C7
2	A	501	MYR	C11-C10-C9-C8
2	A	501	MYR	C4-C5-C6-C7
2	C	501	MYR	C11-C10-C9-C8
2	A	501	MYR	C6-C7-C8-C9
2	C	501	MYR	C6-C7-C8-C9
2	D	501	MYR	C11-C12-C13-C14
3	A	502	KMU	C13-C10-C12-C15
3	A	502	KMU	C13-C10-C12-C19
3	C	502	KMU	C13-C10-C12-C15
3	C	502	KMU	C13-C10-C12-C19
3	D	502	KMU	C13-C10-C12-C19
2	C	501	MYR	C9-C10-C11-C12
2	A	501	MYR	C9-C10-C11-C12
2	D	501	MYR	C4-C5-C6-C7
3	A	502	KMU	O9-C10-C12-C15

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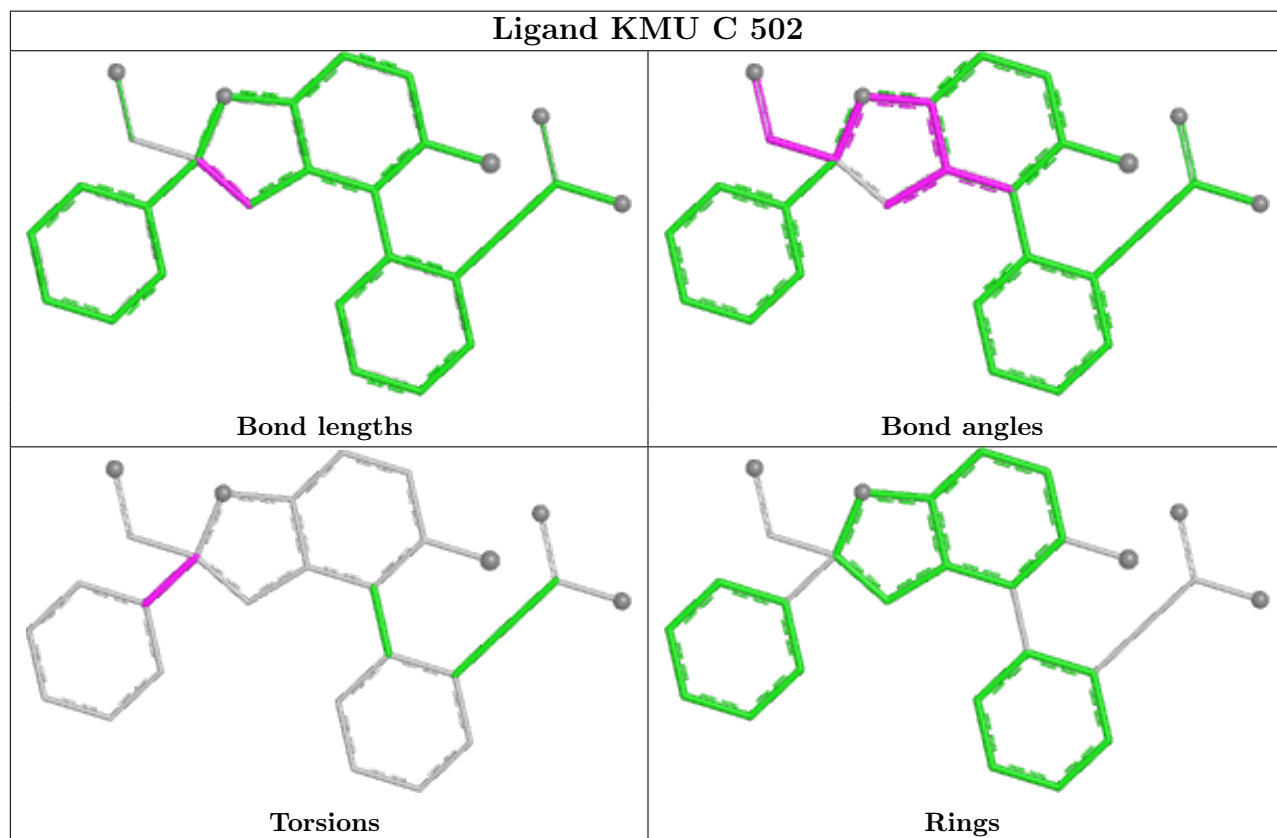
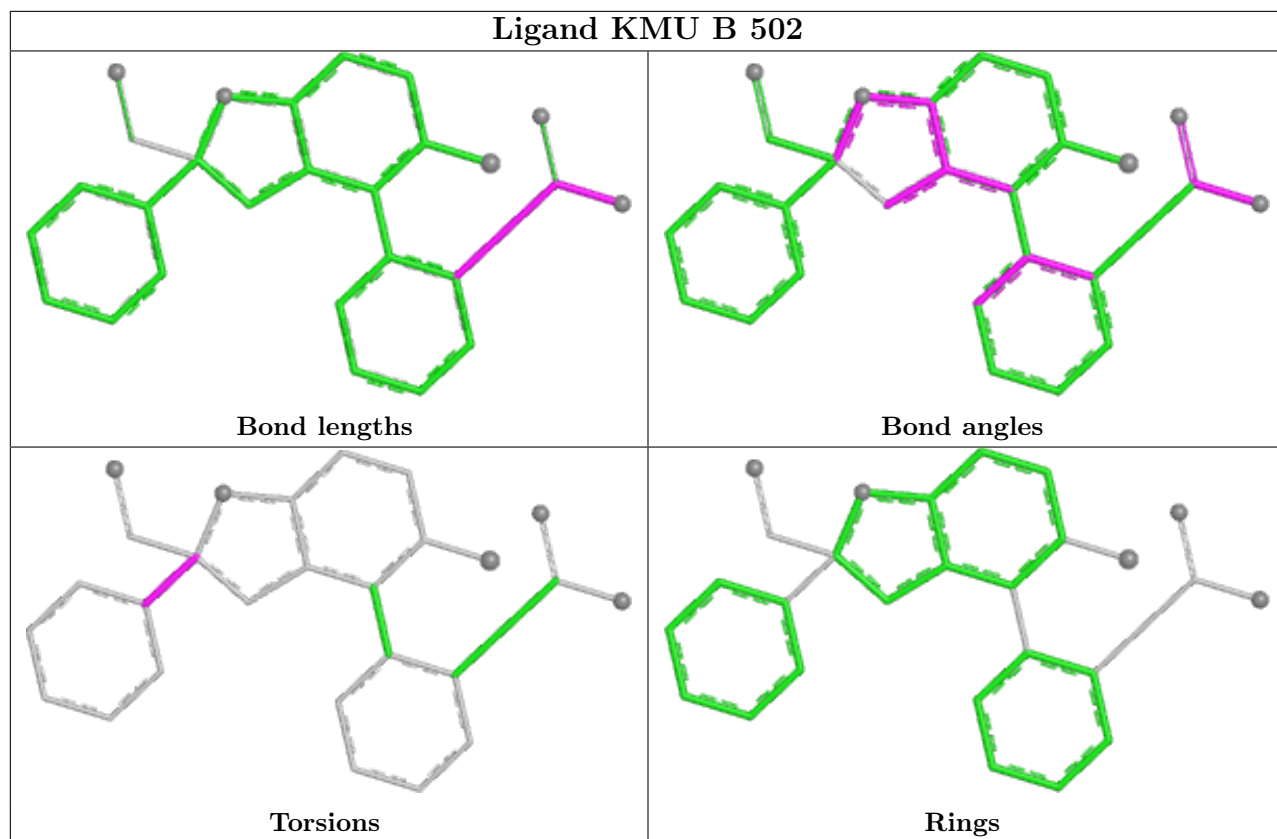
Mol	Chain	Res	Type	Atoms
3	C	502	KMU	O9-C10-C12-C15
3	C	502	KMU	O9-C10-C12-C19
3	B	502	KMU	C13-C10-C12-C15
3	B	502	KMU	C13-C10-C12-C19
2	B	501	MYR	C4-C5-C6-C7

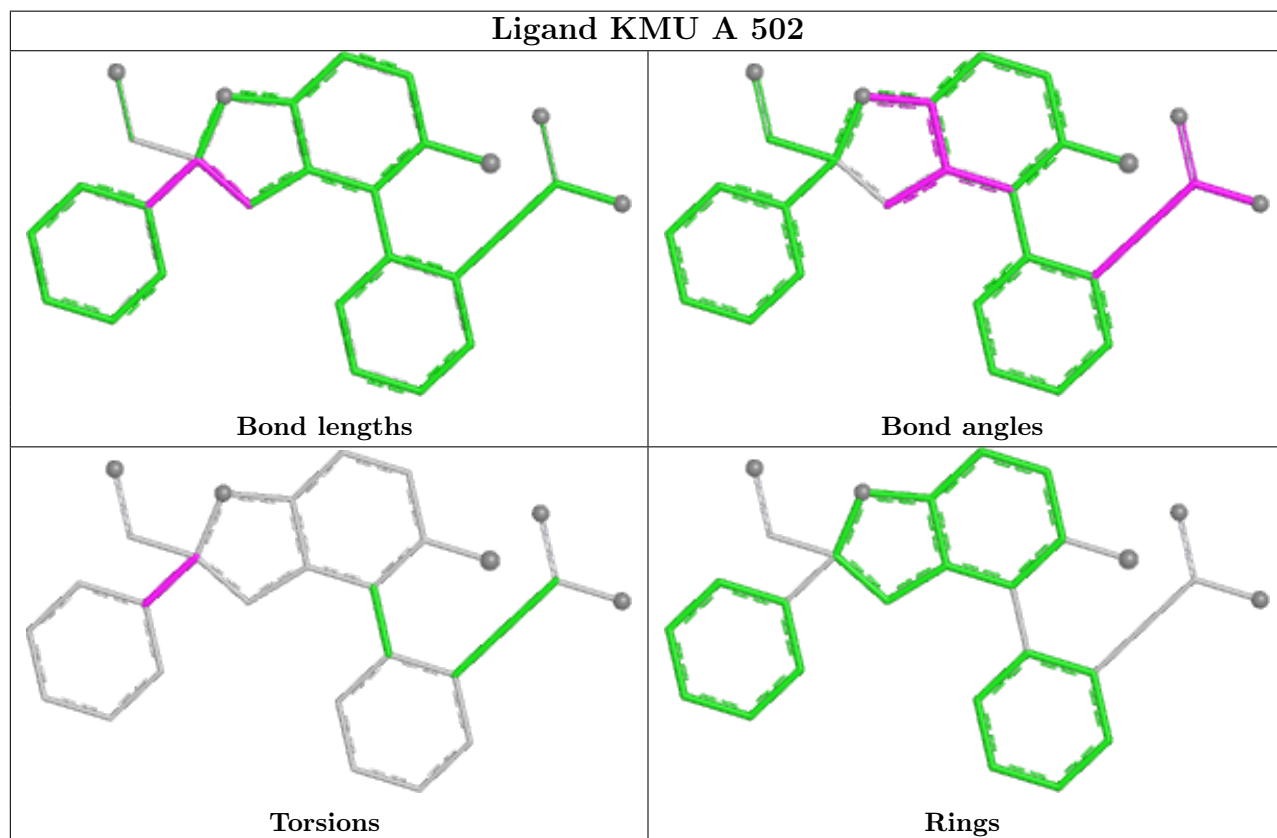
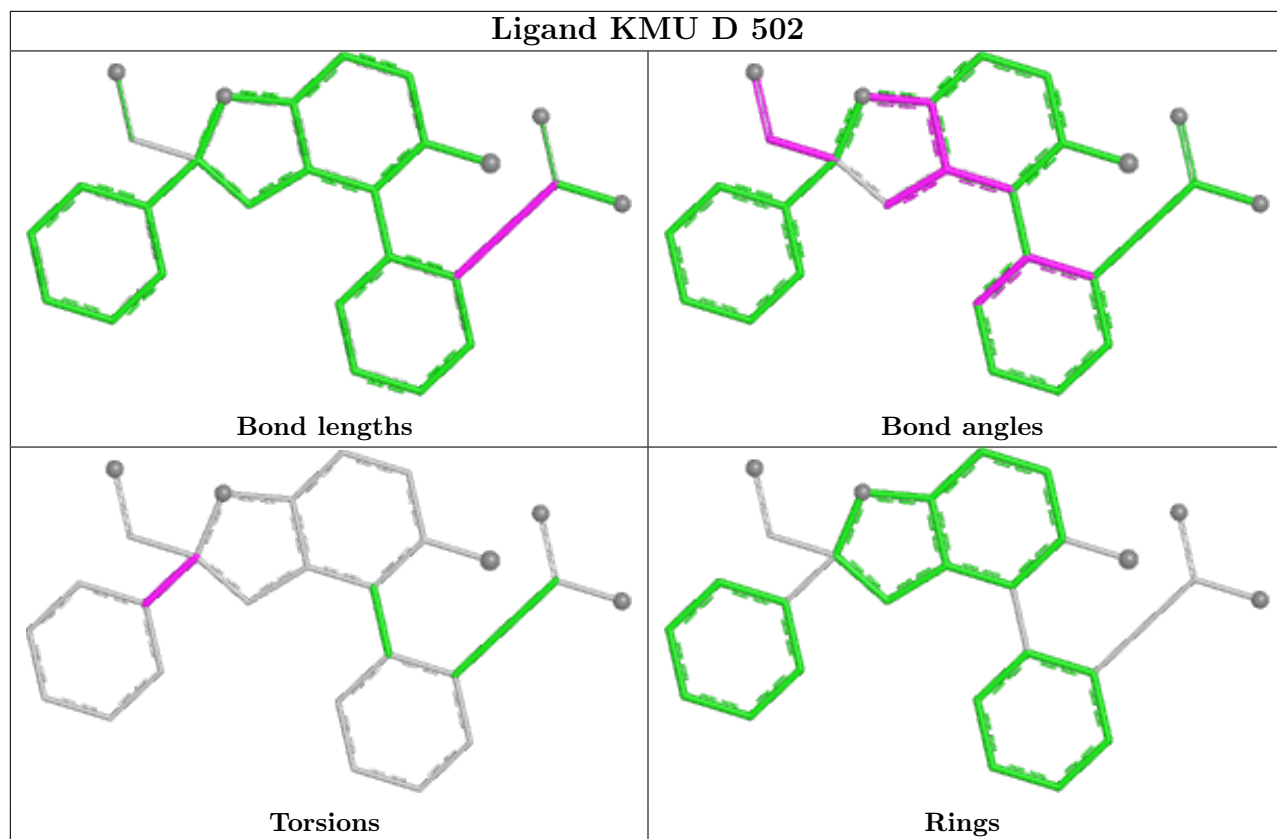
There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	KMU	1	0
3	D	502	KMU	1	0
2	C	501	MYR	3	0
2	B	501	MYR	8	0
2	A	501	MYR	3	0
2	D	501	MYR	8	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	209/222 (94%)	-0.02	8 (3%) 40 36	15, 32, 50, 78	0
1	B	209/222 (94%)	0.02	7 (3%) 46 41	18, 35, 54, 71	0
1	C	206/222 (92%)	0.04	11 (5%) 26 22	18, 35, 55, 65	0
1	D	208/222 (93%)	-0.02	8 (3%) 40 36	13, 32, 53, 69	0
All	All	832/888 (93%)	0.00	34 (4%) 37 32	13, 33, 54, 78	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	423	HIS	5.9
1	D	254	THR	5.0
1	D	422	GLU	4.4
1	D	424	GLY	4.2
1	B	435	ASP	4.2
1	B	423	HIS	4.1
1	C	260	ASP	4.1
1	A	435	ASP	3.9
1	A	260	ASP	3.6
1	C	423	HIS	3.5
1	D	262	PRO	3.5
1	A	306	THR	3.4
1	A	423	HIS	3.3
1	A	380	HIS	3.1
1	C	435	ASP	3.0
1	B	422	GLU	3.0
1	B	262	PRO	3.0
1	D	421	SER	2.9
1	C	380	HIS	2.9
1	A	382	PRO	2.8
1	C	424	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	254	THR	2.8
1	C	261	PRO	2.7
1	D	253	GLN	2.7
1	C	281	GLY	2.6
1	C	276	PRO	2.5
1	C	420	THR	2.4
1	A	307	ILE	2.3
1	B	280	GLY	2.3
1	C	310	GLY	2.3
1	C	422	GLU	2.2
1	D	306	THR	2.1
1	B	306	THR	2.1
1	A	308	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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.

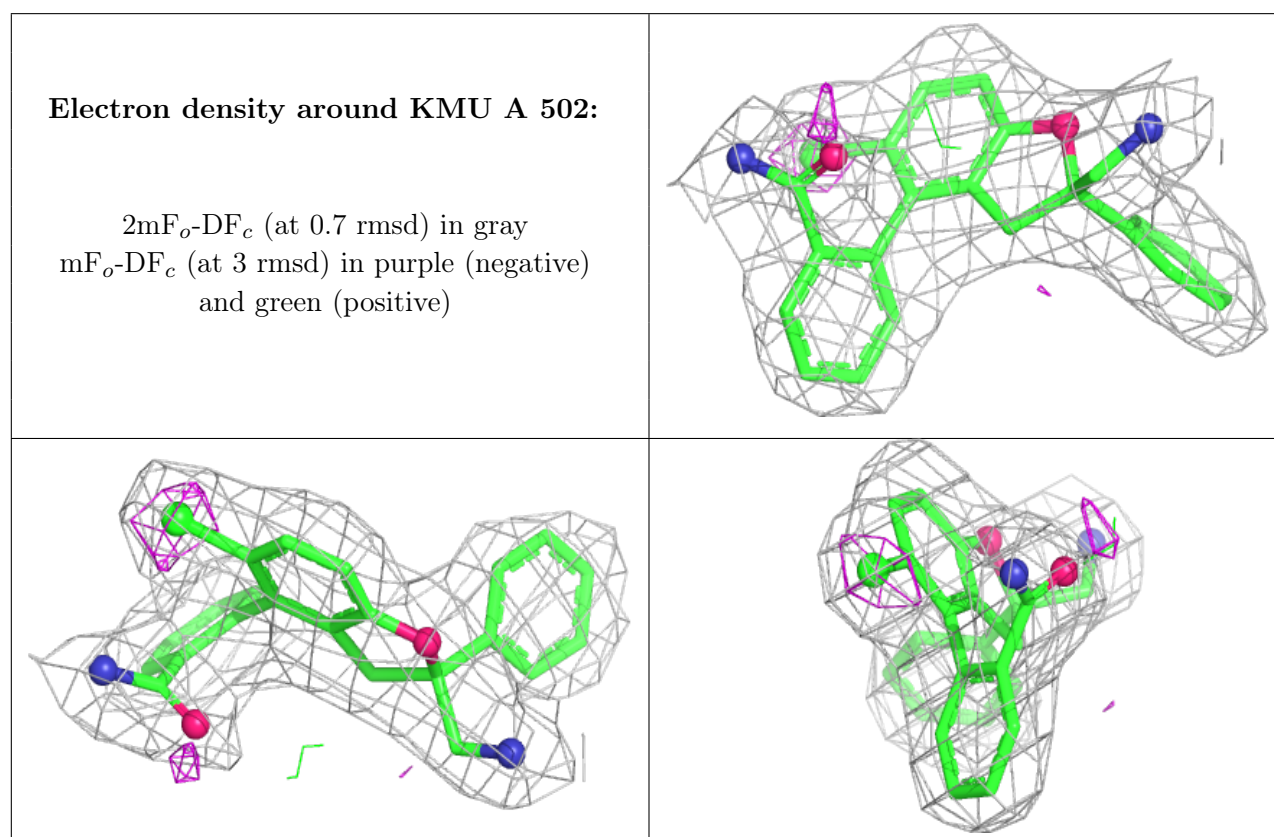
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	A	505	5/5	0.82	0.29	108,108,109,109	0
4	PO4	C	505	5/5	0.82	0.24	94,94,94,94	0
2	MYR	D	501	15/16	0.87	0.26	29,32,35,37	0
2	MYR	B	501	15/16	0.88	0.23	23,29,35,36	0
2	MYR	A	501	15/16	0.90	0.25	27,29,33,33	0
4	PO4	A	504	5/5	0.90	0.26	85,85,85,85	0
4	PO4	D	504	5/5	0.91	0.23	93,93,94,94	0
2	MYR	C	501	15/16	0.92	0.27	21,23,27,27	0
4	PO4	C	504	5/5	0.92	0.28	61,61,62,62	0
3	KMU	A	502	27/27	0.94	0.16	25,27,29,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	KMU	B	502	27/27	0.95	0.14	27,29,30,33	0
4	PO4	C	503	5/5	0.96	0.36	57,57,57,58	0
4	PO4	A	503	5/5	0.96	0.14	52,52,52,53	0
3	KMU	C	502	27/27	0.96	0.20	38,39,41,41	0
4	PO4	D	503	5/5	0.96	0.12	53,53,54,54	0
3	KMU	D	502	27/27	0.96	0.15	19,22,26,26	0

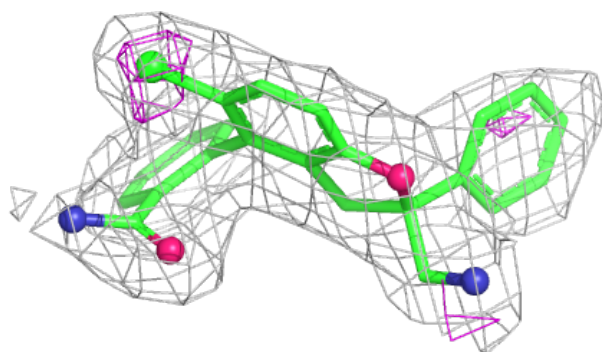
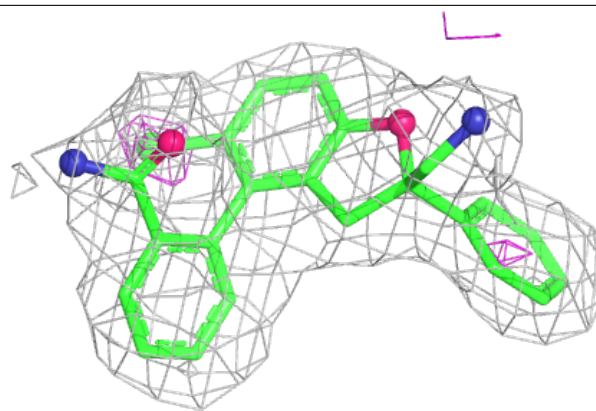
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



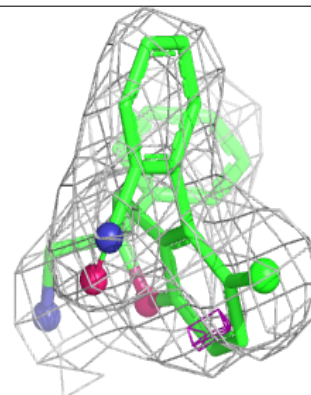
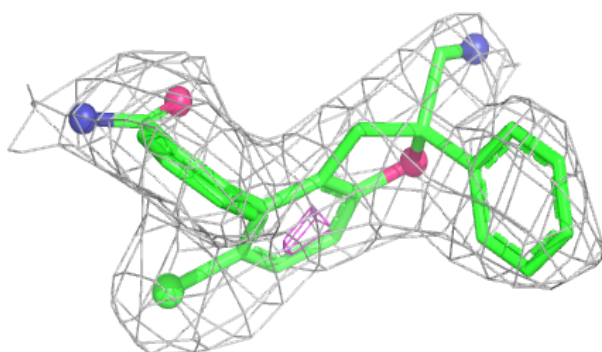
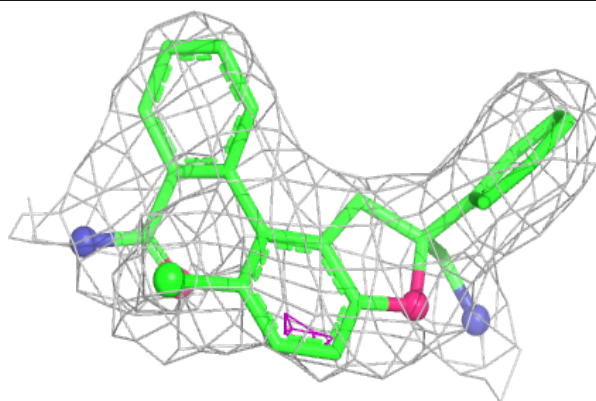


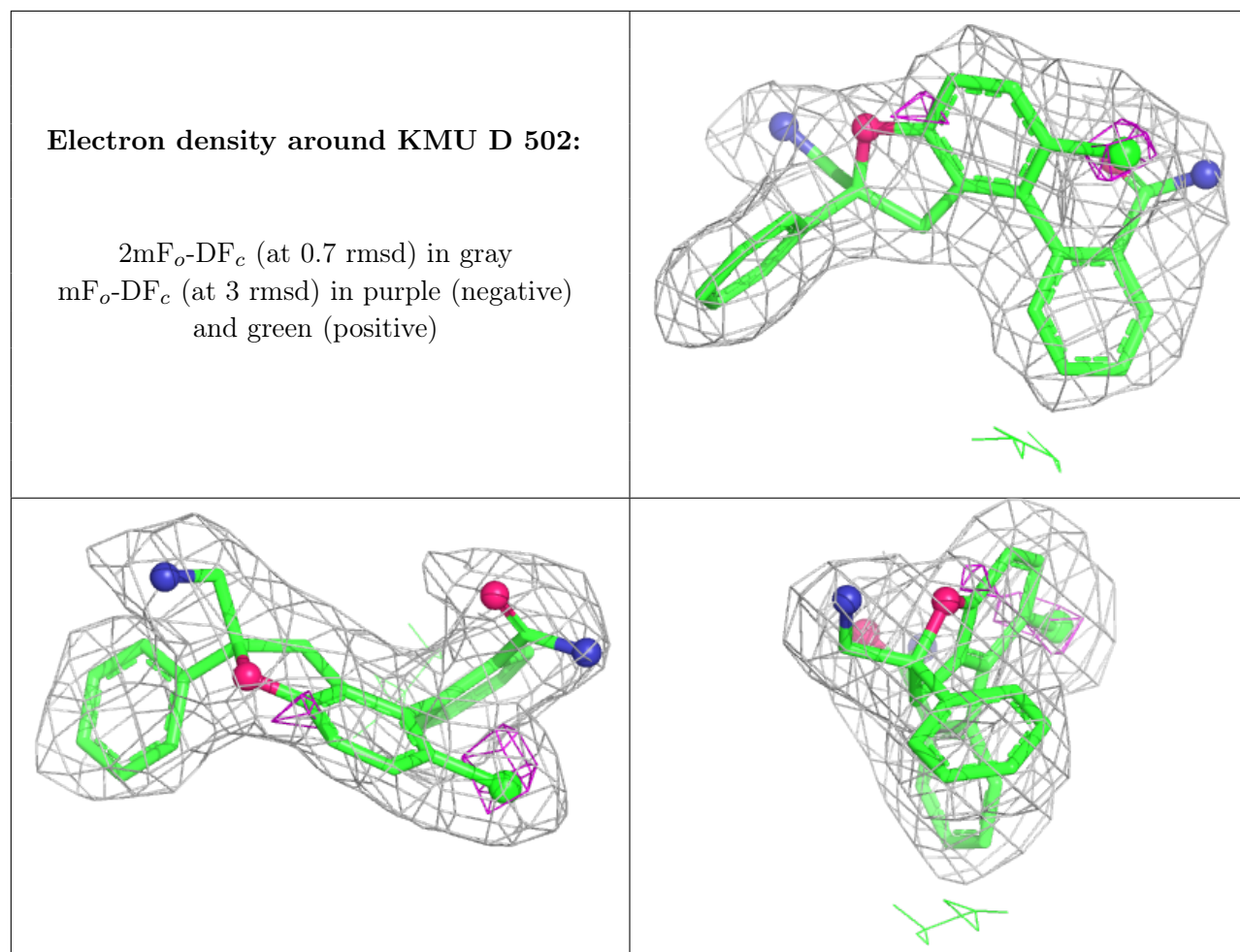
**Electron density around KMU B 502:**

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

**Electron density around KMU C 502:**

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





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.