



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 8, 2025 – 01:11 pm BST

PDB ID : 9HB8 / pdb\_00009hb8  
Title : Crystal structure of human tryptophan hydroxylase 2 in complex with inhibitor KM-06-098  
Authors : Schuetz, A.; Mallow, K.; Nazare, M.; Specker, E.; Heinemann, U.  
Deposited on : 2024-11-05  
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>.

---

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

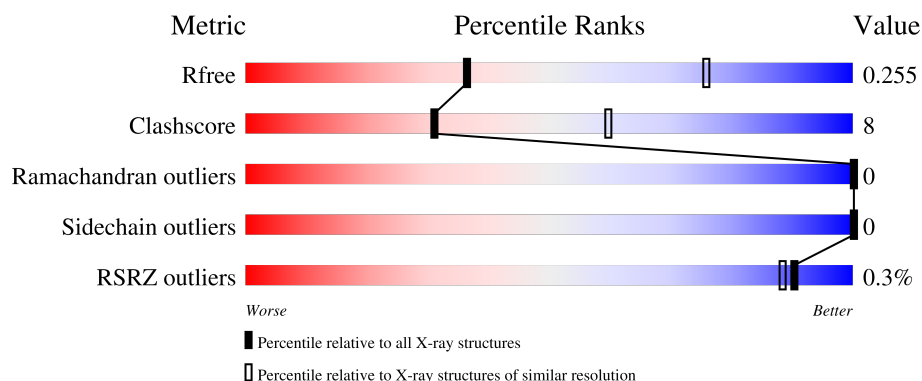
# 1 Overall quality at a glance

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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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	372	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>8%</div> </div> </div>
1	B	372	<div> <div></div> <div>70%</div> <div>19%</div> <div>10%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5565 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 Tryptophan 5-hydroxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2769	1772	461	520	16			
1	B	334	Total	C	N	O	S	0	0	0
			2720	1742	451	511	16			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	initiating methionine	UNP Q8IWU9
A	120	LYS	-	expression tag	UNP Q8IWU9
A	121	HIS	-	expression tag	UNP Q8IWU9
A	122	HIS	-	expression tag	UNP Q8IWU9
A	123	HIS	-	expression tag	UNP Q8IWU9
A	124	HIS	-	expression tag	UNP Q8IWU9
A	125	HIS	-	expression tag	UNP Q8IWU9
A	126	HIS	-	expression tag	UNP Q8IWU9
A	127	HIS	-	expression tag	UNP Q8IWU9
A	128	GLY	-	expression tag	UNP Q8IWU9
A	129	ALA	-	expression tag	UNP Q8IWU9
A	130	ALA	-	expression tag	UNP Q8IWU9
A	131	GLY	-	expression tag	UNP Q8IWU9
A	132	THR	-	expression tag	UNP Q8IWU9
A	133	SER	-	expression tag	UNP Q8IWU9
A	134	LEU	-	expression tag	UNP Q8IWU9
A	135	TYR	-	expression tag	UNP Q8IWU9
A	136	LYS	-	expression tag	UNP Q8IWU9
A	137	LYS	-	expression tag	UNP Q8IWU9
A	138	ALA	-	expression tag	UNP Q8IWU9
A	139	GLY	-	expression tag	UNP Q8IWU9
A	140	GLU	-	expression tag	UNP Q8IWU9
A	141	ASN	-	expression tag	UNP Q8IWU9
A	142	LEU	-	expression tag	UNP Q8IWU9
A	143	TYR	-	expression tag	UNP Q8IWU9

*Continued on next page...*

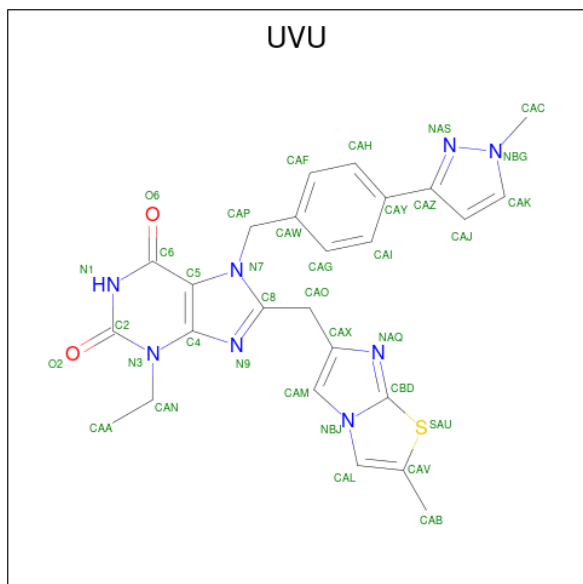
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	PHE	-	expression tag	UNP Q8IWU9
A	145	GLN	-	expression tag	UNP Q8IWU9
A	146	GLY	-	expression tag	UNP Q8IWU9
A	147	SER	-	expression tag	UNP Q8IWU9
B	119	MET	-	initiating methionine	UNP Q8IWU9
B	120	LYS	-	expression tag	UNP Q8IWU9
B	121	HIS	-	expression tag	UNP Q8IWU9
B	122	HIS	-	expression tag	UNP Q8IWU9
B	123	HIS	-	expression tag	UNP Q8IWU9
B	124	HIS	-	expression tag	UNP Q8IWU9
B	125	HIS	-	expression tag	UNP Q8IWU9
B	126	HIS	-	expression tag	UNP Q8IWU9
B	127	HIS	-	expression tag	UNP Q8IWU9
B	128	GLY	-	expression tag	UNP Q8IWU9
B	129	ALA	-	expression tag	UNP Q8IWU9
B	130	ALA	-	expression tag	UNP Q8IWU9
B	131	GLY	-	expression tag	UNP Q8IWU9
B	132	THR	-	expression tag	UNP Q8IWU9
B	133	SER	-	expression tag	UNP Q8IWU9
B	134	LEU	-	expression tag	UNP Q8IWU9
B	135	TYR	-	expression tag	UNP Q8IWU9
B	136	LYS	-	expression tag	UNP Q8IWU9
B	137	LYS	-	expression tag	UNP Q8IWU9
B	138	ALA	-	expression tag	UNP Q8IWU9
B	139	GLY	-	expression tag	UNP Q8IWU9
B	140	GLU	-	expression tag	UNP Q8IWU9
B	141	ASN	-	expression tag	UNP Q8IWU9
B	142	LEU	-	expression tag	UNP Q8IWU9
B	143	TYR	-	expression tag	UNP Q8IWU9
B	144	PHE	-	expression tag	UNP Q8IWU9
B	145	GLN	-	expression tag	UNP Q8IWU9
B	146	GLY	-	expression tag	UNP Q8IWU9
B	147	SER	-	expression tag	UNP Q8IWU9

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

- Molecule 3 is 3-ethyl-8-[(2-methylimidazo[2,1-b][1,3]thiazol-6-yl)methyl]-7-[[4-(1-methylpyrazol-3-yl)phenyl]methyl]purine-2,6-dione (CCD ID: UVU) (formula: C<sub>25</sub>H<sub>24</sub>N<sub>8</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			36	25	8	2	1		
3	B	1	Total	C	N	O	S	0	0
			36	25	8	2	1		

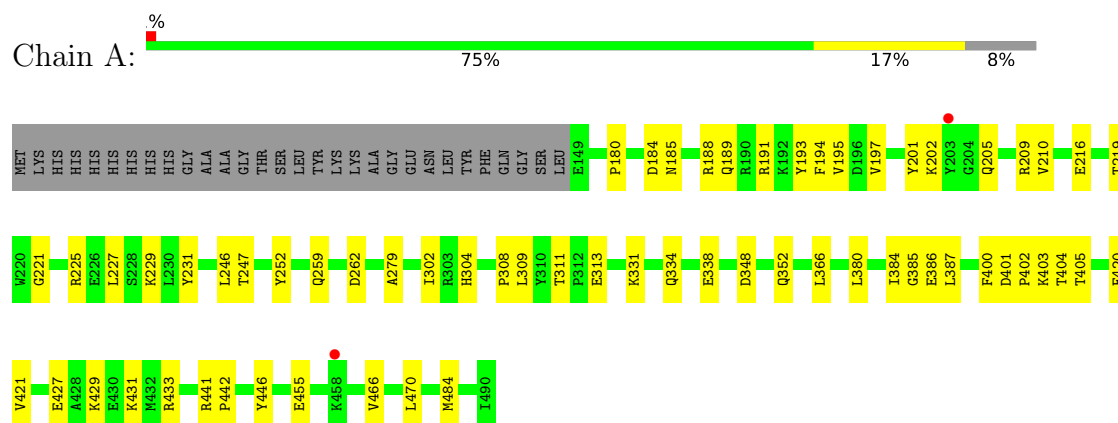
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		

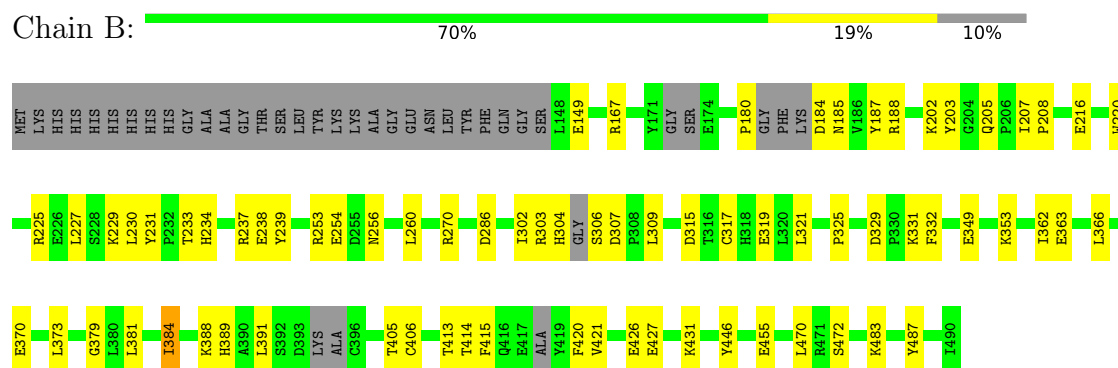
### 3 Residue-property plots [i](#)

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: Tryptophan 5-hydroxylase 2



#### • Molecule 1: Tryptophan 5-hydroxylase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.51Å 94.11Å 87.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.90 47.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.05-2.90) 99.4 (47.05-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.209 , 0.249 0.219 , 0.255	Depositor DCC
$R_{free}$ test set	954 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.5	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: FE, UVU

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	0.34	0/2839	0.81	0/3841
1	B	0.35	0/2784	0.94	6/3762 (0.2%)
All	All	0.34	0/5623	0.87	6/7603 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ILE	N-CA-C	7.71	117.82	110.42
1	B	149	GLU	N-CA-C	6.30	117.84	110.41
1	B	389	HIS	N-CA-C	5.47	117.32	111.36
1	B	413	THR	N-CA-C	5.39	119.80	112.04
1	B	233	THR	N-CA-C	5.07	116.88	111.36
1	B	270	ARG	N-CA-C	5.00	116.81	111.36

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	2769	0	2699	45	0
1	B	2720	0	2646	47	0
2	A	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	36	0	0	0	0
3	B	36	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	5565	0	5345	88	0

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

All (88) 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:A:366:LEU:HB2	1:A:421:VAL:HG22	1.66	0.77
1:A:219:THR:HG23	1:A:308:PRO:HB3	1.68	0.75
1:A:201:TYR:HA	1:A:205:GLN:NE2	2.04	0.73
1:A:400:PHE:O	1:A:431:LYS:NZ	2.24	0.70
1:B:225:ARG:HD3	1:B:254:GLU:OE2	1.98	0.64
1:A:201:TYR:HA	1:A:205:GLN:HE21	1.64	0.62
1:B:216:GLU:HB3	1:B:302:ILE:HG13	1.82	0.62
1:A:446:TYR:HB3	1:A:455:GLU:HB2	1.83	0.60
1:B:234:HIS:CD2	1:B:391:LEU:HD22	2.38	0.59
1:A:227:LEU:HB3	1:A:231:TYR:CZ	2.38	0.58
1:A:216:GLU:HB3	1:A:302:ILE:HG13	1.86	0.58
1:B:227:LEU:HB3	1:B:231:TYR:CZ	2.39	0.57
1:A:338:GLU:OE1	1:A:433:ARG:NH1	2.38	0.56
1:A:191:ARG:O	1:A:195:VAL:HG23	2.05	0.56
1:A:380:LEU:HD23	1:A:386:GLU:HG2	1.88	0.56
1:B:315:ASP:O	1:B:319:GLU:HG2	2.06	0.55
1:B:167:ARG:HD2	1:B:286:ASP:OD2	2.06	0.55
1:B:230:LEU:HB3	1:B:234:HIS:ND1	2.21	0.55
1:B:353:LYS:HE3	1:B:406:CYS:SG	2.47	0.55
1:B:234:HIS:HD2	1:B:391:LEU:HD22	1.70	0.54
1:B:253:ARG:HH21	1:B:256:ASN:HD22	1.56	0.54
1:A:209:ARG:NH2	1:A:262:ASP:OD1	2.32	0.54
1:A:225:ARG:O	1:A:229:LYS:HG3	2.06	0.54
1:B:185:ASN:HA	1:B:188:ARG:HG3	1.89	0.54
1:B:180:PRO:O	1:B:184:ASP:N	2.41	0.53
1:B:331:LYS:HD2	1:B:426:GLU:HG2	1.91	0.53
1:B:220:TRP:NE1	1:B:256:ASN:O	2.41	0.53
1:B:349:GLU:O	1:B:353:LYS:HG3	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:O	1:B:379:GLY:N	2.41	0.52
1:A:246:LEU:HB3	1:A:252:TYR:CD1	2.45	0.52
1:B:227:LEU:HD22	1:B:381:LEU:O	2.10	0.51
1:A:194:PHE:CE1	1:A:210:VAL:HG11	2.45	0.51
1:A:401:ASP:HB3	1:A:404:THR:OG1	2.10	0.51
1:A:433:ARG:NH1	1:B:472:SER:HB3	2.26	0.51
1:A:442:PRO:HA	1:B:487:TYR:CE1	2.46	0.50
1:B:427:GLU:OE2	1:B:431:LYS:HD2	2.12	0.50
1:A:185:ASN:O	1:A:189:GLN:HG3	2.12	0.49
1:B:202:LYS:HG2	1:B:203:TYR:N	2.26	0.49
1:B:229:LYS:HB2	1:B:230:LEU:HD12	1.95	0.49
1:B:225:ARG:O	1:B:229:LYS:HG2	2.13	0.49
1:A:405:THR:HG23	1:A:420:PHE:CZ	2.48	0.49
1:B:405:THR:HG23	1:B:420:PHE:CE2	2.47	0.48
1:B:309:LEU:HD13	1:B:384:ILE:HD11	1.96	0.48
1:B:384:ILE:O	1:B:388:LYS:HG3	2.14	0.48
1:A:195:VAL:HG13	1:A:279:ALA:HB1	1.96	0.48
1:B:446:TYR:HB3	1:B:455:GLU:HB2	1.96	0.47
1:A:309:LEU:HD13	1:A:384:ILE:HD11	1.98	0.46
1:A:338:GLU:HG3	1:A:429:LYS:HG3	1.97	0.46
1:B:227:LEU:HD12	1:B:321:LEU:HD13	1.98	0.46
1:B:239:TYR:CE2	1:B:325:PRO:HG2	2.51	0.46
1:A:311:THR:HG22	1:A:313:GLU:H	1.80	0.46
1:B:180:PRO:HB2	1:B:304:HIS:ND1	2.32	0.45
1:A:441:ARG:O	1:B:483:LYS:HD3	2.16	0.45
1:B:202:LYS:O	1:B:205:GLN:HG2	2.16	0.45
1:A:210:VAL:O	1:A:259:GLN:NE2	2.50	0.45
1:A:384:ILE:HG13	1:A:385:GLY:N	2.32	0.45
1:B:207:ILE:HG21	1:B:260:LEU:HB2	1.99	0.45
1:B:253:ARG:HH21	1:B:256:ASN:ND2	2.14	0.45
1:A:180:PRO:HB2	1:A:304:HIS:ND1	2.32	0.44
1:B:237:ARG:HH11	1:B:370:GLU:HG3	1.82	0.44
1:B:239:TYR:CE2	1:B:381:LEU:HD13	2.52	0.44
1:B:187:TYR:OH	1:B:302:ILE:O	2.35	0.44
1:B:306:SER:OG	1:B:307:ASP:N	2.50	0.44
1:A:366:LEU:O	1:A:421:VAL:HA	2.18	0.43
1:A:401:ASP:OD2	1:A:403:LYS:HE2	2.18	0.43
1:A:334:GLN:HB3	1:A:429:LYS:HD2	1.99	0.43
1:A:470:LEU:HD22	1:B:470:LEU:HD22	1.99	0.43
1:B:238:GLU:HG2	1:B:329:ASP:OD2	2.18	0.43
1:B:332:PHE:CZ	1:B:362:ILE:HD12	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HA	1:A:252:TYR:HB2	2.01	0.43
1:B:237:ARG:NH1	1:B:370:GLU:HG3	2.34	0.43
1:B:366:LEU:O	1:B:421:VAL:HA	2.19	0.42
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.84	0.42
1:A:202:LYS:O	1:A:205:GLN:HG2	2.19	0.42
1:A:348:ASP:O	1:A:352:GLN:HG2	2.18	0.42
1:B:303:ARG:HH11	1:B:317:CYS:HB2	1.84	0.42
1:A:466:VAL:O	1:A:470:LEU:HG	2.20	0.42
1:A:380:LEU:O	1:A:387:LEU:HB2	2.19	0.42
1:A:427:GLU:O	1:A:431:LYS:HG3	2.19	0.42
1:A:193:TYR:O	1:A:197:VAL:HG23	2.19	0.42
1:A:331:LYS:HD3	1:A:331:LYS:HA	1.81	0.42
1:B:414:THR:HG22	1:B:415:PHE:N	2.35	0.42
1:A:402:PRO:HG2	1:A:431:LYS:O	2.20	0.41
1:A:184:ASP:O	1:A:188:ARG:HG3	2.20	0.41
1:A:380:LEU:CD2	1:A:386:GLU:HG2	2.50	0.41
1:A:221:GLY:O	1:A:225:ARG:HG3	2.21	0.41
1:A:484:MET:HB2	1:A:484:MET:HE3	1.72	0.41
1:B:207:ILE:HA	1:B:208:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/372 (91%)	334 (98%)	6 (2%)	0	100	100
1	B	322/372 (87%)	316 (98%)	6 (2%)	0	100	100
All	All	662/744 (89%)	650 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	303/326 (93%)	303 (100%)	0	100	100
1	B	300/326 (92%)	300 (100%)	0	100	100
All	All	603/652 (92%)	603 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	256	ASN
1	B	205	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	UVU	B	502	2	30,41,41	3.36	9 (30%)	31,61,61	2.81	10 (32%)
3	UVU	A	502	2	30,41,41	3.26	9 (30%)	31,61,61	2.75	11 (35%)

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	UVU	B	502	2	-	2/12/14/14	0/6/6/6
3	UVU	A	502	2	-	2/12/14/14	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	UVU	CAV-SAU	-10.25	1.59	1.73
3	B	502	UVU	CAY-CAZ	-9.79	1.33	1.48
3	A	502	UVU	CAY-CAZ	-9.67	1.33	1.48
3	A	502	UVU	CAV-SAU	-9.51	1.60	1.73
3	A	502	UVU	CAJ-CAZ	-6.08	1.32	1.40
3	B	502	UVU	CAJ-CAZ	-6.03	1.32	1.40
3	B	502	UVU	C2-N3	-4.89	1.34	1.37
3	A	502	UVU	C2-N3	-4.83	1.34	1.37
3	B	502	UVU	CAP-CAW	-4.65	1.40	1.51
3	A	502	UVU	CAP-CAW	-4.50	1.40	1.51
3	A	502	UVU	C5-C6	-4.39	1.34	1.45
3	B	502	UVU	C5-C6	-4.37	1.34	1.45
3	B	502	UVU	C4-N3	-3.09	1.34	1.39
3	A	502	UVU	C4-N3	-2.90	1.35	1.39
3	A	502	UVU	CAK-CAJ	-2.55	1.33	1.37
3	B	502	UVU	CAK-CAJ	-2.53	1.33	1.37
3	A	502	UVU	CAM-CAX	-2.10	1.33	1.36
3	B	502	UVU	CAM-CAX	-2.03	1.33	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	UVU	C6-N1-C2	-9.56	118.53	127.35
3	A	502	UVU	C6-N1-C2	-9.50	118.59	127.35
3	A	502	UVU	CAV-CAL-NBJ	6.45	114.52	107.89
3	B	502	UVU	CAV-CAL-NBJ	6.08	114.14	107.89
3	B	502	UVU	CAB-CAV-SAU	4.59	124.94	119.88
3	B	502	UVU	CAJ-CAZ-CAY	-4.52	124.55	128.77
3	A	502	UVU	CAJ-CAZ-CAY	-4.24	124.81	128.77
3	A	502	UVU	CAB-CAV-SAU	4.22	124.53	119.88
3	B	502	UVU	CAC-NBG-NAS	4.04	125.25	120.50
3	A	502	UVU	CAC-NBG-NAS	3.99	125.19	120.50
3	B	502	UVU	CAY-CAZ-NAS	3.11	125.88	120.93
3	A	502	UVU	CAY-CAZ-NAS	3.02	125.73	120.93
3	B	502	UVU	O2-C2-N3	-2.88	120.21	122.00
3	B	502	UVU	CAK-NBG-NAS	-2.87	110.06	111.73
3	A	502	UVU	CAK-NBG-NAS	-2.78	110.12	111.73
3	A	502	UVU	O2-C2-N3	-2.41	120.50	122.00
3	B	502	UVU	N1-C2-N3	2.39	119.64	115.39
3	A	502	UVU	N1-C2-N3	2.32	119.51	115.39
3	B	502	UVU	CAJ-CAK-NBG	2.10	107.85	106.81
3	A	502	UVU	O6-C6-N1	-2.06	118.22	120.65
3	A	502	UVU	CAJ-CAK-NBG	2.04	107.82	106.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

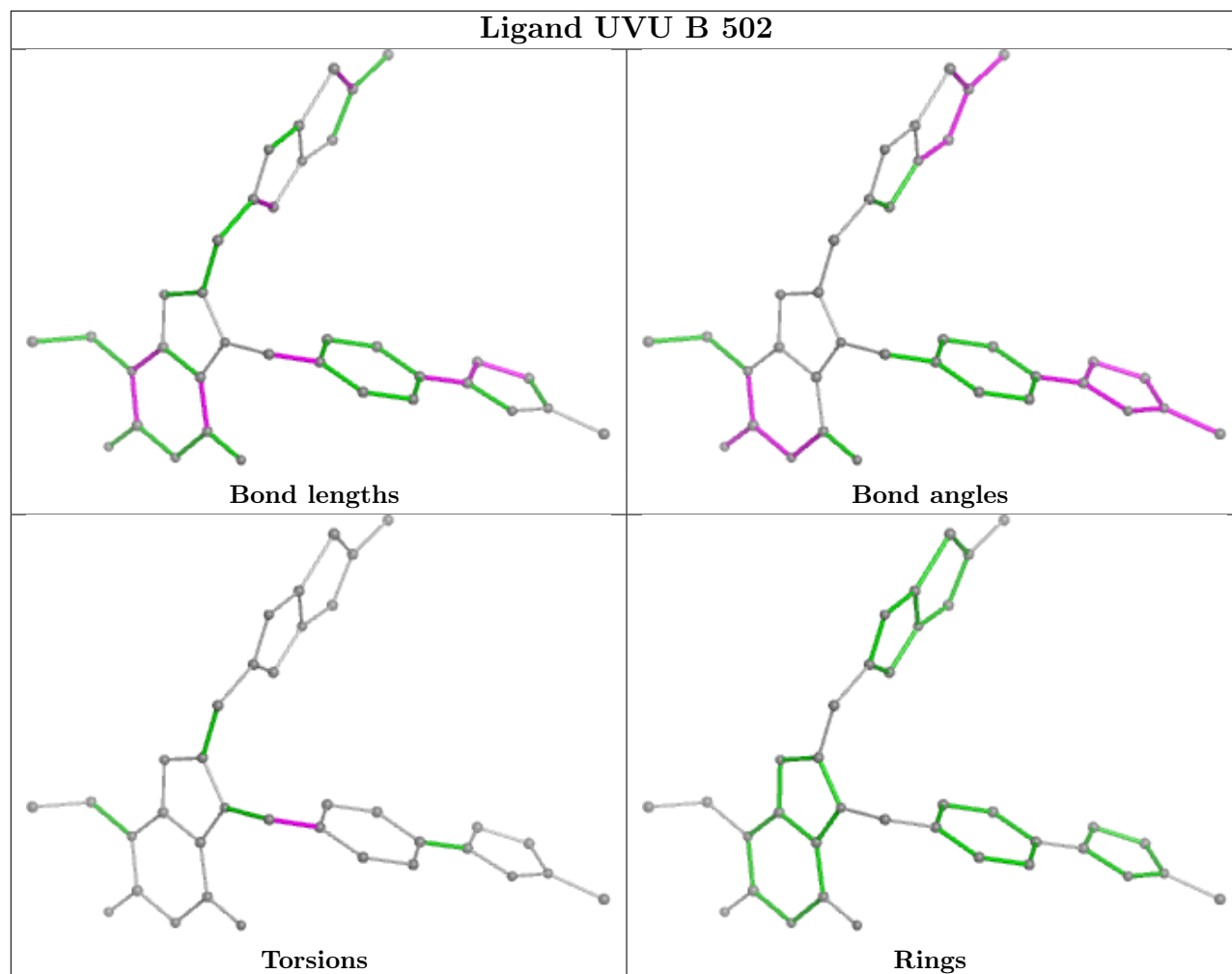
Mol	Chain	Res	Type	Atoms
3	A	502	UVU	N7-CAP-CAW-CAF
3	A	502	UVU	N7-CAP-CAW-CAG
3	B	502	UVU	N7-CAP-CAW-CAG
3	B	502	UVU	N7-CAP-CAW-CAF

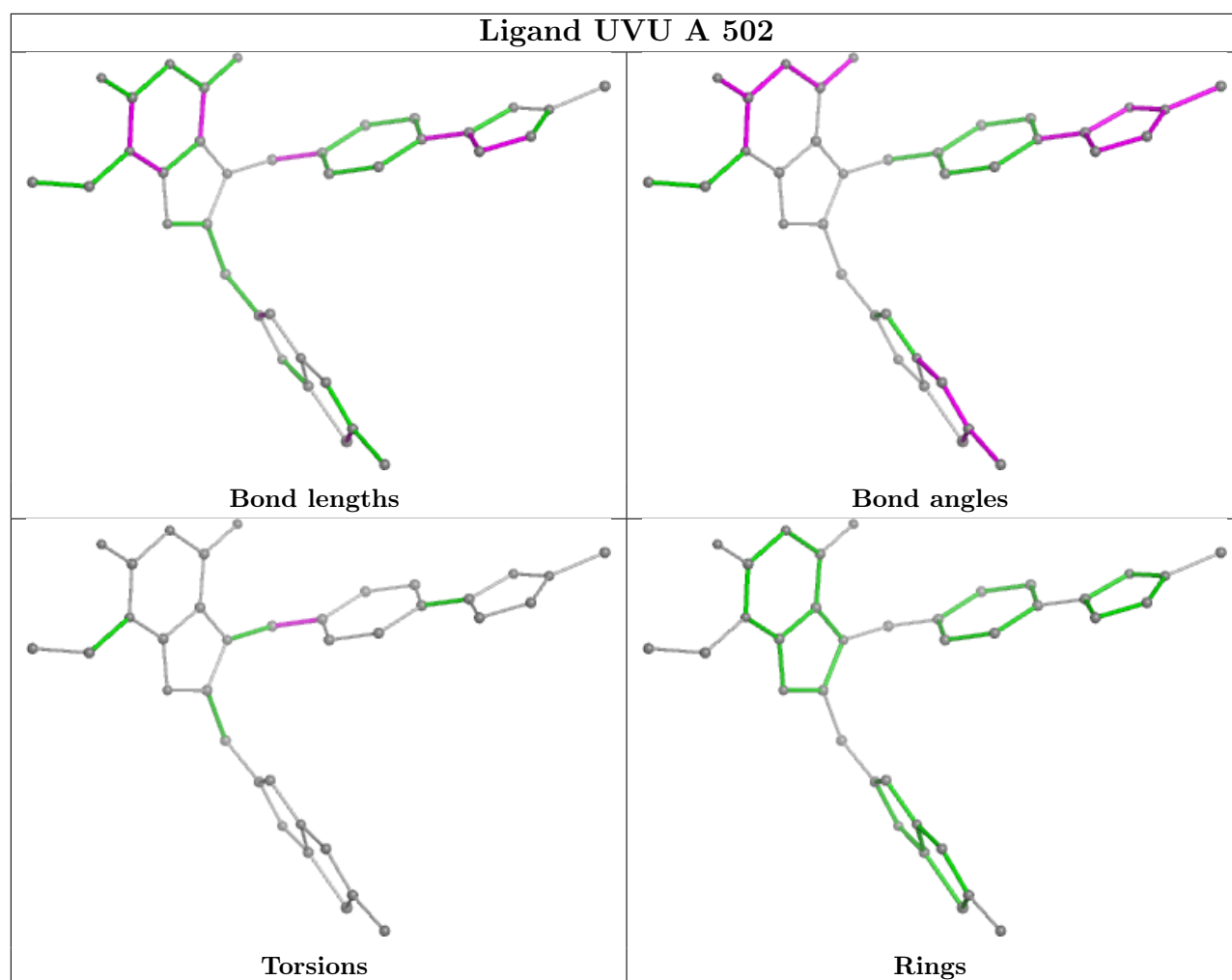
There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 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	342/372 (91%)	-0.43	2 (0%) 85 82	53, 86, 144, 186	0
1	B	334/372 (89%)	-0.27	0 100 100	56, 120, 178, 213	0
All	All	676/744 (90%)	-0.35	2 (0%) 90 88	53, 101, 173, 213	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	TYR	2.2
1	A	458	LYS	2.2

### 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, 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
3	UVU	B	502	36/36	0.86	0.11	120,136,141,149	0
3	UVU	A	502	36/36	0.95	0.09	72,101,107,108	0
2	FE	B	501	1/1	0.99	0.04	105,105,105,105	0

*Continued on next page...*

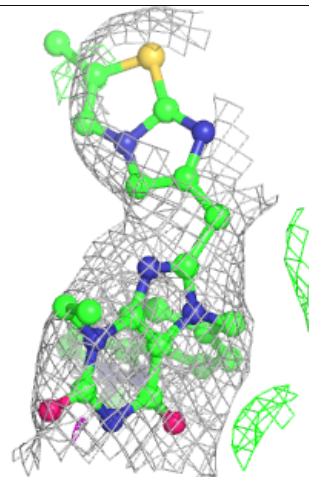
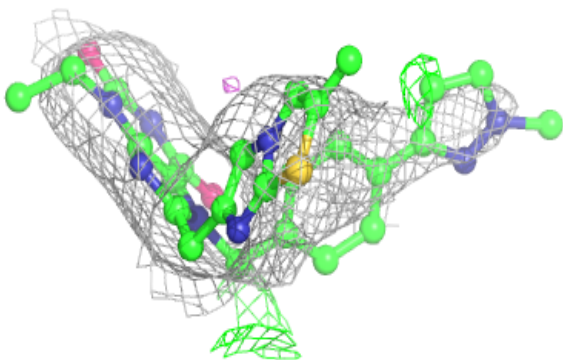
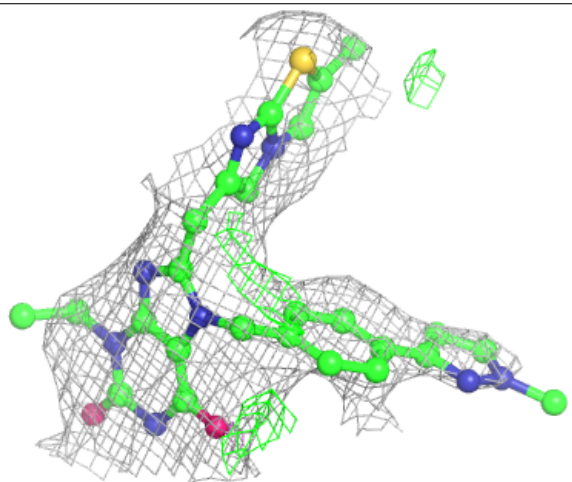
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	A	501	1/1	1.00	0.03	79,79,79,79	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.

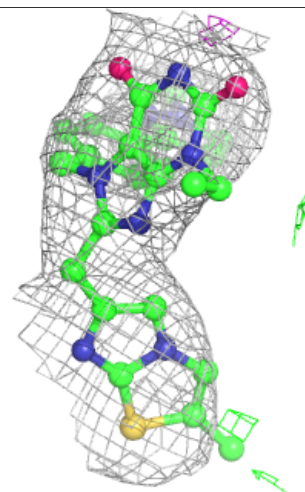
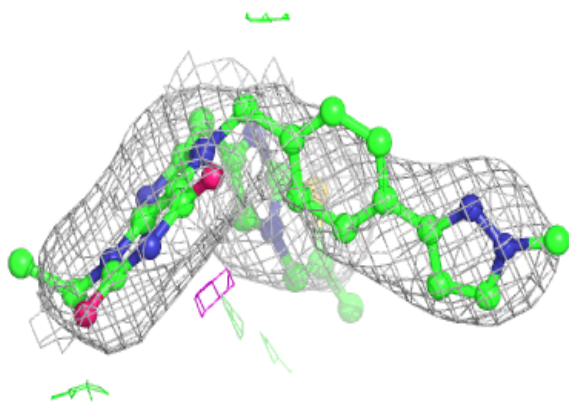
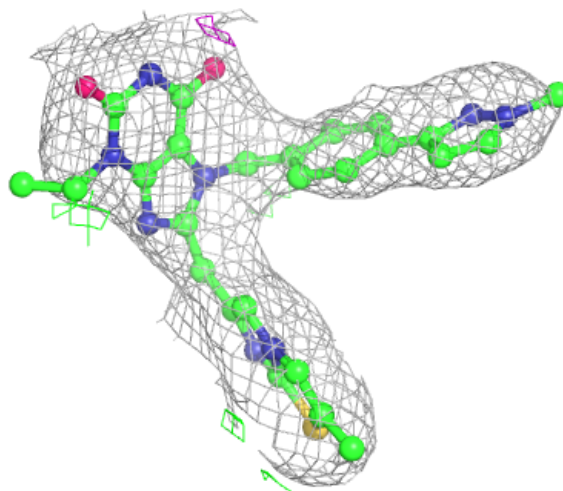
#### Electron density around UVU B 502:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UVU A 502:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.