



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2024 – 12:04 PM EDT

PDB ID : 8UF6  
Title : Structure of Trek-1(K2P2.1) with ML336  
Authors : Lolicato, M.; Mondal, A.; Minor, D.L.  
Deposited on : 2023-10-03  
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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

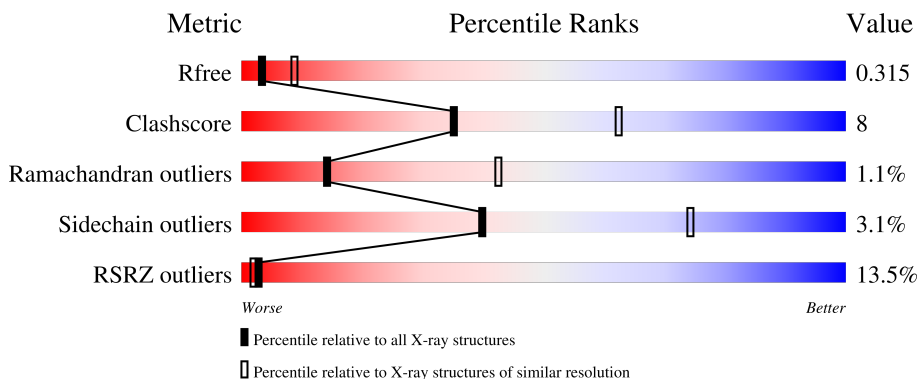
# 1 Overall quality at a glance

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	287	 13% 71% 22% 7%
1	B	287	 13% 77% 20% 7%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4487 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 Potassium channel subfamily K member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2099	1403	331	361	4	0	0	0
1	B	282	2178	1449	346	378	5	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

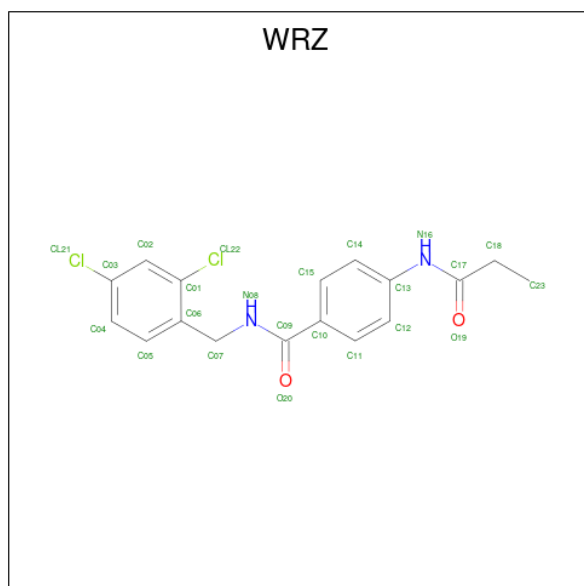
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ARG	LYS	engineered mutation	UNP P97438
A	85	GLU	GLN	engineered mutation	UNP P97438
A	86	LYS	THR	engineered mutation	UNP P97438
A	88	LEU	ILE	engineered mutation	UNP P97438
A	89	ARG	ALA	engineered mutation	UNP P97438
A	90	ALA	GLN	engineered mutation	UNP P97438
A	92	PRO	ALA	engineered mutation	UNP P97438
A	95	SER	ASN	engineered mutation	UNP P97438
A	96	ASP	SER	engineered mutation	UNP P97438
A	97	GLN	THR	engineered mutation	UNP P97438
A	119	ALA	ASN	engineered mutation	UNP P97438
A	300	ALA	SER	engineered mutation	UNP P97438
A	306	ALA	GLU	engineered mutation	UNP P97438
B	84	ARG	LYS	engineered mutation	UNP P97438
B	85	GLU	GLN	engineered mutation	UNP P97438
B	86	LYS	THR	engineered mutation	UNP P97438
B	88	LEU	ILE	engineered mutation	UNP P97438
B	89	ARG	ALA	engineered mutation	UNP P97438
B	90	ALA	GLN	engineered mutation	UNP P97438
B	92	PRO	ALA	engineered mutation	UNP P97438
B	95	SER	ASN	engineered mutation	UNP P97438
B	96	ASP	SER	engineered mutation	UNP P97438
B	97	GLN	THR	engineered mutation	UNP P97438
B	119	ALA	ASN	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438

*Continued on next page...*

Continued from previous page...

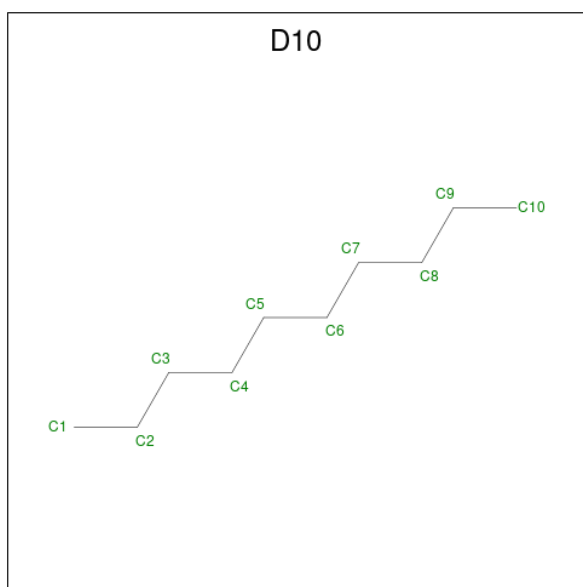
Chain	Residue	Modelled	Actual	Comment	Reference
B	306	ALA	GLU	engineered mutation	UNP P97438

- Molecule 2 is N-[(2,4-dichlorophenyl)methyl]-4-propanamidobenzamide (three-letter code: WRZ) (formula:  $C_{17}H_{16}Cl_2N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	23	17	2	2	2	0	0
2	B	1	23	17	2	2	2	0	0

- Molecule 3 is DECANE (three-letter code: D10) (formula:  $C_{10}H_{22}$ ).

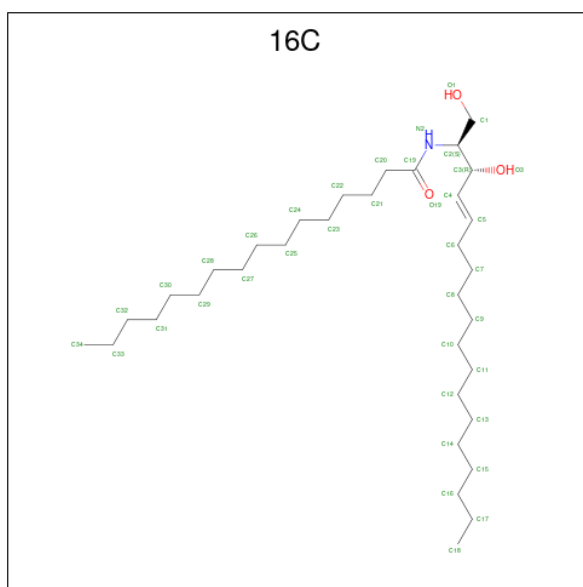


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

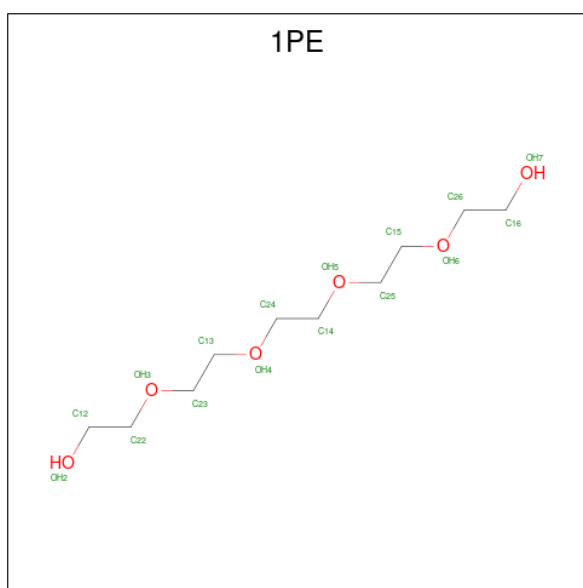
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total K 3 3	0	0
4	B	3	Total K 3 3	0	0

- Molecule 5 is N-((E,2S,3R)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL)PALMITAMIDE (three-letter code: 16C) (formula: C<sub>34</sub>H<sub>67</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	A	1	38	34	1	3	0	0
5	B	1	38	34	1	3	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).

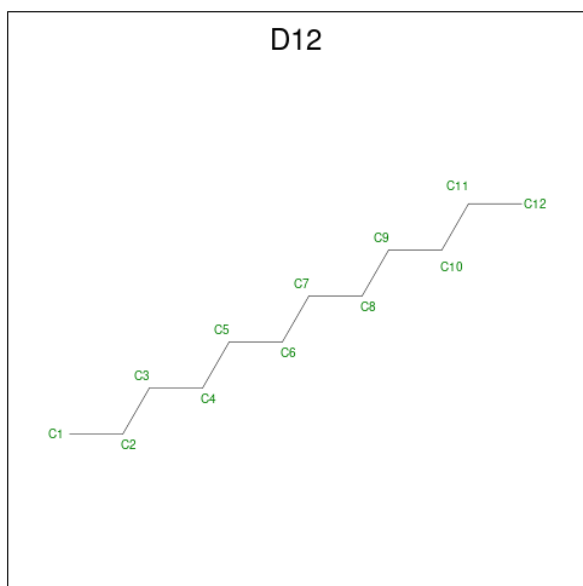


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	16	10	6	0	0

- Molecule 7 is CADMIUM ION (three-letter code: CD) (formula: Cd).

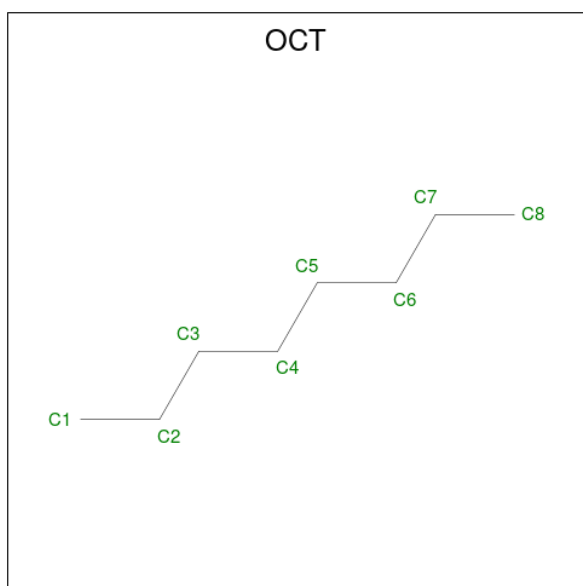
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Cd 2 2	0	0

- Molecule 8 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).



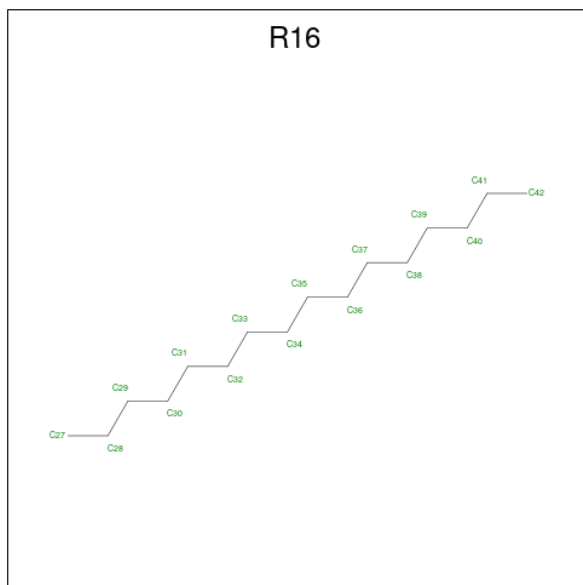
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 12 12	0	0

- Molecule 9 is N-OCTANE (three-letter code: OCT) (formula:  $C_8H_{18}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 8 8	0	0
9	B	1	Total C 8 8	0	0

- Molecule 10 is HEXADECANE (three-letter code: R16) (formula: C<sub>16</sub>H<sub>34</sub>).



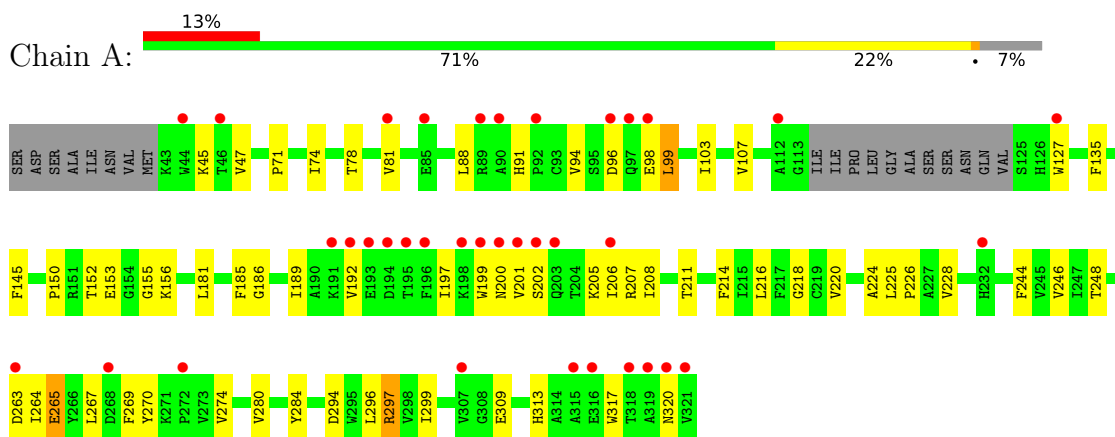
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 16 16	0	0



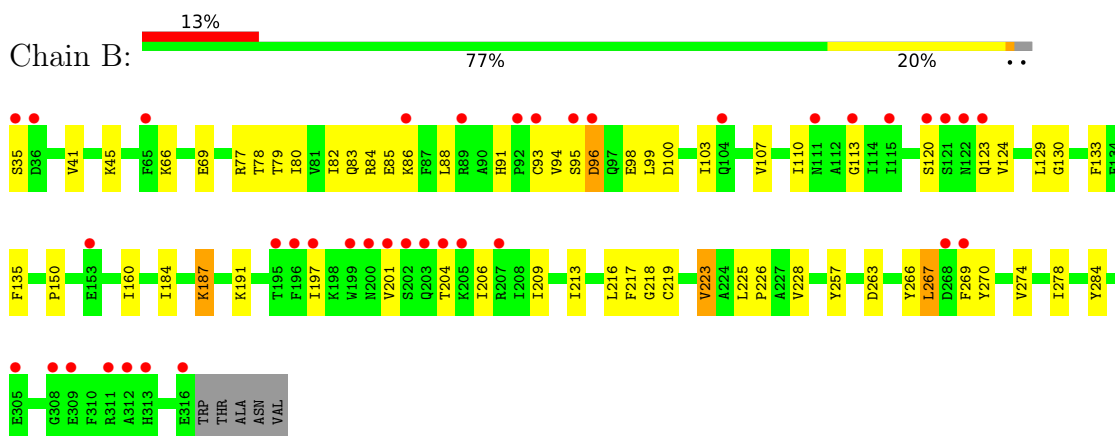
### 3 Residue-property plots [i](#)

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: Potassium channel subfamily K member 2



- Molecule 1: Potassium channel subfamily K member 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.95Å 118.60Å 130.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.90 – 2.90 14.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (14.90-2.90) 98.9 (14.90-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.267 , 0.313 0.264 , 0.315	Depositor DCC
$R_{free}$ test set	1113 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.7	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 106.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D12, OCT, 1PE, R16, D10, K, CD, WRZ, 16C

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	0.29	0/2152	0.53	0/2927
1	B	0.29	0/2231	0.54	0/3034
All	All	0.29	0/4383	0.53	0/5961

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

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	2099	0	2146	38	0
1	B	2178	0	2217	40	0
2	A	23	0	0	0	0
2	B	23	0	0	1	0
3	A	20	0	44	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	38	0	67	1	0
5	B	38	0	67	0	0
6	B	16	0	22	1	0
7	B	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	12	0	26	0	0
9	B	16	0	36	0	0
10	B	16	0	34	0	0
All	All	4487	0	4659	75	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 (75) 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:B:79:THR:HA	1:B:82:ILE:HG12	1.58	0.84
1:A:181:LEU:HD11	1:A:280:VAL:HG13	1.72	0.71
1:B:94:VAL:HG12	1:B:96:ASP:H	1.53	0.71
1:A:152:THR:HG23	1:A:155:GLY:H	1.59	0.66
1:B:206:ILE:O	1:B:209:ILE:HG13	1.95	0.66
1:B:197:ILE:HD13	1:B:201:VAL:HG11	1.80	0.63
1:B:82:ILE:HG13	1:B:83:GLN:N	2.14	0.62
1:A:244:PHE:O	1:A:248:THR:HG23	2.03	0.59
1:B:184:ILE:O	1:B:187:LYS:HG3	2.04	0.58
1:B:267:LEU:H	1:B:267:LEU:HD12	1.68	0.58
1:B:130:GLY:HA3	6:B:402:1PE:H232	1.85	0.58
1:A:202:SER:O	1:A:206:ILE:HG13	2.04	0.57
1:B:82:ILE:O	1:B:86:LYS:HG3	2.06	0.55
1:B:82:ILE:HG13	1:B:83:GLN:H	1.71	0.55
1:B:41:VAL:O	1:B:45:LYS:HG3	2.06	0.54
1:A:270:TYR:O	1:A:274:VAL:HG22	2.08	0.54
1:A:45:LYS:C	1:A:47:VAL:H	2.11	0.54
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.42	0.54
1:A:78:THR:HA	1:A:81:VAL:HG22	1.90	0.53
1:A:99:LEU:O	1:A:103:ILE:HG12	2.08	0.52
1:A:309:GLU:O	1:A:313:HIS:ND1	2.39	0.52
1:A:294:ASP:HA	1:A:297:ARG:HG2	1.92	0.52
1:B:99:LEU:O	1:B:103:ILE:HG23	2.10	0.51
1:B:123:GLN:HG2	1:B:124:VAL:H	1.75	0.51
1:A:91:HIS:O	1:A:94:VAL:HG12	2.09	0.51
5:A:407:16C:O3	5:A:407:16C:O1	2.29	0.51
1:B:77:ARG:O	1:B:80:ILE:HG22	2.11	0.50
1:A:207:ARG:O	1:A:211:THR:HG23	2.11	0.49
1:B:85:GLU:HA	1:B:88:LEU:HB2	1.95	0.49
1:B:95:SER:OG	1:B:98:GLU:HB2	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:CA	1:B:82:ILE:HG12	2.35	0.49
1:A:103:ILE:O	1:A:107:VAL:HG22	2.13	0.49
1:A:135:PHE:CZ	1:A:150:PRO:HD3	2.48	0.48
1:A:152:THR:HG22	1:B:69:GLU:OE2	2.14	0.48
1:B:270:TYR:O	1:B:274:VAL:HG23	2.13	0.48
2:B:401:WRZ:N08	2:B:401:WRZ:CL22	2.83	0.48
1:B:100:ASP:O	1:B:103:ILE:HG12	2.13	0.47
1:A:205:LYS:O	1:A:208:ILE:HG12	2.13	0.47
1:B:78:THR:O	1:B:82:ILE:HG23	2.14	0.47
1:A:181:LEU:HD11	1:A:280:VAL:CG1	2.44	0.46
1:A:185:PHE:CZ	1:A:214:PHE:HB2	2.50	0.46
1:B:213:ILE:HG23	1:B:217:PHE:HD2	1.80	0.46
1:B:225:LEU:O	1:B:228:VAL:HG22	2.16	0.46
1:A:88:LEU:HD11	1:A:96:ASP:HA	1.98	0.46
1:A:246:VAL:HG11	1:B:160:ILE:HG23	1.97	0.46
1:B:107:VAL:HA	1:B:110:ILE:HG22	1.97	0.46
1:A:199:TRP:O	1:A:201:VAL:N	2.49	0.45
1:B:100:ASP:HA	1:B:103:ILE:HG12	1.98	0.45
1:A:220:VAL:HA	1:A:224:ALA:HB3	1.97	0.45
1:B:218:GLY:HA3	1:B:284:TYR:CZ	2.53	0.44
1:B:82:ILE:HB	1:B:86:LYS:NZ	2.33	0.44
1:A:98:GLU:OE1	1:B:91:HIS:NE2	2.48	0.44
1:B:191:LYS:HD3	1:B:191:LYS:HA	1.55	0.44
1:B:129:LEU:O	1:B:133:PHE:HB2	2.17	0.43
1:A:313:HIS:O	1:A:317:TRP:HB2	2.18	0.43
1:B:225:LEU:N	1:B:226:PRO:HD2	2.34	0.43
1:B:267:LEU:C	1:B:269:PHE:H	2.21	0.43
1:B:218:GLY:HA3	1:B:284:TYR:CE1	2.53	0.43
1:A:296:LEU:O	1:A:299:ILE:HG13	2.18	0.43
1:A:127:TRP:O	1:B:66:LYS:HG3	2.19	0.42
1:A:218:GLY:HA3	1:A:284:TYR:CE1	2.54	0.42
1:A:216:LEU:O	1:A:220:VAL:HG13	2.20	0.42
1:A:145:PHE:CE1	1:A:248:THR:HG22	2.54	0.42
1:A:225:LEU:N	1:A:226:PRO:HD2	2.34	0.42
1:A:225:LEU:HA	1:A:228:VAL:HG22	2.02	0.42
1:A:297:ARG:HE	1:A:297:ARG:HB2	1.48	0.41
1:B:84:ARG:O	1:B:88:LEU:HG	2.21	0.41
1:B:219:CYS:O	1:B:223:VAL:HG13	2.19	0.41
1:A:186:GLY:O	1:A:189:ILE:HG13	2.21	0.41
1:B:213:ILE:HD13	1:B:216:LEU:HD21	2.02	0.41
1:A:263:ASP:O	1:A:265:GLU:N	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:O	1:A:320:ASN:HB3	2.21	0.40
1:A:71:PRO:O	1:A:74:ILE:HG13	2.22	0.40
1:A:156:LYS:NZ	1:B:257:TYR:OH	2.54	0.40
1:A:267:LEU:C	1:A:269:PHE:H	2.24	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	264/287 (92%)	250 (95%)	11 (4%)	3 (1%)	14	42
1	B	280/287 (98%)	258 (92%)	19 (7%)	3 (1%)	14	42
All	All	544/574 (95%)	508 (93%)	30 (6%)	6 (1%)	14	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	B	113	GLY
1	B	266	TYR
1	A	265	GLU
1	B	120	SER
1	A	264	ILE

### 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	219/236 (93%)	214 (98%)	5 (2%)	50	80
1	B	226/236 (96%)	217 (96%)	9 (4%)	31	65
All	All	445/472 (94%)	431 (97%)	14 (3%)	40	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	153	GLU
1	A	192	VAL
1	A	197	ILE
1	A	297	ARG
1	B	35	SER
1	B	93	CYS
1	B	96	ASP
1	B	187	LYS
1	B	204	THR
1	B	223	VAL
1	B	263	ASP
1	B	267	LEU
1	B	278	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	16C	A	407	-	36,37,37	1.58	5 (13%)	37,39,39	1.00	2 (5%)
9	OCT	B	411	-	7,7,7	0.26	0	6,6,6	0.18	0
9	OCT	B	410	-	7,7,7	0.27	0	6,6,6	0.18	0
10	R16	B	412	-	15,15,15	0.30	0	14,14,14	0.89	0
2	WRZ	B	401	1	24,24,24	1.64	4 (16%)	32,32,32	2.20	13 (40%)
3	D10	A	403	-	9,9,9	0.32	0	8,8,8	0.76	0
3	D10	A	402	-	9,9,9	0.31	0	8,8,8	0.79	0
2	WRZ	A	401	1	24,24,24	1.64	4 (16%)	32,32,32	2.09	11 (34%)
6	1PE	B	402	-	15,15,15	0.15	0	14,14,14	0.07	0
5	16C	B	409	-	36,37,37	1.58	5 (13%)	37,39,39	1.07	2 (5%)
8	D12	B	408	-	11,11,11	0.26	0	10,10,10	0.27	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	16C	A	407	-	-	21/40/40/40	-
9	OCT	B	411	-	-	2/5/5/5	-
9	OCT	B	410	-	-	0/5/5/5	-
10	R16	B	412	-	-	6/13/13/13	-
2	WRZ	B	401	1	-	2/15/15/15	0/2/2/2
3	D10	A	403	-	-	0/7/7/7	-
3	D10	A	402	-	-	3/7/7/7	-
2	WRZ	A	401	1	-	2/15/15/15	0/2/2/2
6	1PE	B	402	-	-	5/13/13/13	-
5	16C	B	409	-	-	13/40/40/40	-
8	D12	B	408	-	-	2/9/9/9	-



All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	407	16C	C19-N2	6.81	1.48	1.34
5	B	409	16C	C19-N2	6.71	1.48	1.34
2	A	401	WRZ	C09-N08	4.79	1.44	1.33
2	B	401	WRZ	C09-N08	4.57	1.43	1.33
2	A	401	WRZ	C17-N16	4.21	1.44	1.35
2	B	401	WRZ	C17-N16	4.19	1.44	1.35
5	B	409	16C	C3-C4	3.50	1.56	1.50
5	A	407	16C	C3-C4	3.43	1.55	1.50
5	B	409	16C	C20-C19	2.67	1.56	1.51
2	A	401	WRZ	C01-CL22	2.59	1.79	1.73
5	B	409	16C	O19-C19	-2.58	1.18	1.23
2	B	401	WRZ	C01-CL22	2.55	1.79	1.73
5	A	407	16C	O19-C19	-2.52	1.18	1.23
5	A	407	16C	C20-C19	2.50	1.56	1.51
5	A	407	16C	O3-C3	-2.44	1.38	1.43
5	B	409	16C	O3-C3	-2.35	1.39	1.43
2	A	401	WRZ	O19-C17	-2.05	1.19	1.23
2	B	401	WRZ	O19-C17	-2.01	1.19	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	WRZ	C06-C07-N08	-7.20	97.84	113.03
2	A	401	WRZ	C06-C07-N08	-6.75	98.79	113.03
2	B	401	WRZ	C07-C06-C01	-3.66	116.28	121.13
2	A	401	WRZ	C02-C01-C06	-3.48	119.33	122.42
2	B	401	WRZ	C15-C10-C11	3.24	123.20	118.59
2	B	401	WRZ	C07-N08-C09	-3.23	114.16	121.81
2	A	401	WRZ	C15-C10-C11	3.12	123.04	118.59
2	B	401	WRZ	C02-C01-C06	-3.04	119.72	122.42
2	A	401	WRZ	C07-C06-C01	-2.98	117.18	121.13
2	B	401	WRZ	C14-C15-C10	-2.93	117.37	120.78
2	B	401	WRZ	C05-C06-C01	2.90	121.68	116.91
2	A	401	WRZ	C07-N08-C09	-2.87	115.02	121.81
2	A	401	WRZ	C14-C15-C10	-2.74	117.59	120.78
2	A	401	WRZ	C05-C06-C01	2.71	121.36	116.91
5	B	409	16C	C20-C19-N2	2.53	120.22	115.83
2	B	401	WRZ	C11-C12-C13	-2.41	117.52	120.30
2	B	401	WRZ	C14-C13-C12	2.35	122.25	119.03
2	A	401	WRZ	C23-C18-C17	-2.25	106.14	113.30
2	B	401	WRZ	C02-C01-CL22	2.25	122.12	118.49
2	B	401	WRZ	C14-C13-N16	-2.22	112.94	120.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	WRZ	C14-C13-C12	2.22	122.06	119.03
2	B	401	WRZ	C04-C05-C06	-2.20	118.49	121.39
2	A	401	WRZ	C14-C13-N16	-2.19	113.03	120.40
2	B	401	WRZ	C23-C18-C17	-2.19	106.33	113.30
2	A	401	WRZ	C11-C12-C13	-2.18	117.78	120.30
5	B	409	16C	C2-N2-C19	-2.09	119.96	123.48
5	A	407	16C	C20-C19-N2	2.07	119.43	115.83
5	A	407	16C	C3-C4-C5	-2.03	120.26	124.79

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	16C	O1-C1-C2-C3
5	A	407	16C	O3-C3-C4-C5
5	B	409	16C	C2-C3-C4-C5
6	B	402	1PE	OH4-C13-C23-OH3
6	B	402	1PE	OH5-C14-C24-OH4
6	B	402	1PE	OH7-C16-C26-OH6
10	B	412	R16	C38-C39-C40-C41
5	A	407	16C	C7-C8-C9-C10
10	B	412	R16	C30-C31-C32-C33
5	A	407	16C	C19-C20-C21-C22
5	A	407	16C	C10-C11-C12-C13
5	A	407	16C	C24-C25-C26-C27
5	B	409	16C	C22-C23-C24-C25
10	B	412	R16	C37-C38-C39-C40
5	A	407	16C	C27-C28-C29-C30
5	B	409	16C	C28-C29-C30-C31
5	B	409	16C	C11-C10-C9-C8
5	B	409	16C	C5-C6-C7-C8
3	A	402	D10	C2-C3-C4-C5
5	A	407	16C	C14-C15-C16-C17
10	B	412	R16	C32-C33-C34-C35
5	A	407	16C	C5-C6-C7-C8
5	A	407	16C	C4-C5-C6-C7
10	B	412	R16	C35-C36-C37-C38
5	A	407	16C	C2-C3-C4-C5
5	B	409	16C	O3-C3-C4-C5
8	B	408	D12	C3-C4-C5-C6
2	A	401	WRZ	N16-C17-C18-C23
2	B	401	WRZ	N16-C17-C18-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	409	16C	C9-C10-C11-C12
5	B	409	16C	C15-C16-C17-C18
5	B	409	16C	C4-C5-C6-C7
3	A	402	D10	C1-C2-C3-C4
9	B	411	OCT	C5-C6-C7-C8
2	A	401	WRZ	O19-C17-C18-C23
2	B	401	WRZ	O19-C17-C18-C23
5	A	407	16C	C23-C24-C25-C26
5	B	409	16C	C24-C25-C26-C27
5	A	407	16C	C15-C16-C17-C18
5	B	409	16C	C14-C15-C16-C17
9	B	411	OCT	C4-C5-C6-C7
5	A	407	16C	C21-C22-C23-C24
5	B	409	16C	C21-C22-C23-C24
6	B	402	1PE	C25-C15-OH6-C26
5	A	407	16C	C12-C13-C14-C15
8	B	408	D12	C2-C3-C4-C5
5	B	409	16C	C10-C11-C12-C13
6	B	402	1PE	OH6-C15-C25-OH5
5	A	407	16C	O1-C1-C2-N2
10	B	412	R16	C28-C29-C30-C31
5	A	407	16C	C20-C21-C22-C23
5	A	407	16C	C13-C14-C15-C16
5	A	407	16C	C3-C2-N2-C19
5	A	407	16C	O19-C19-C20-C21
3	A	402	D10	C3-C4-C5-C6
5	A	407	16C	C11-C12-C13-C14

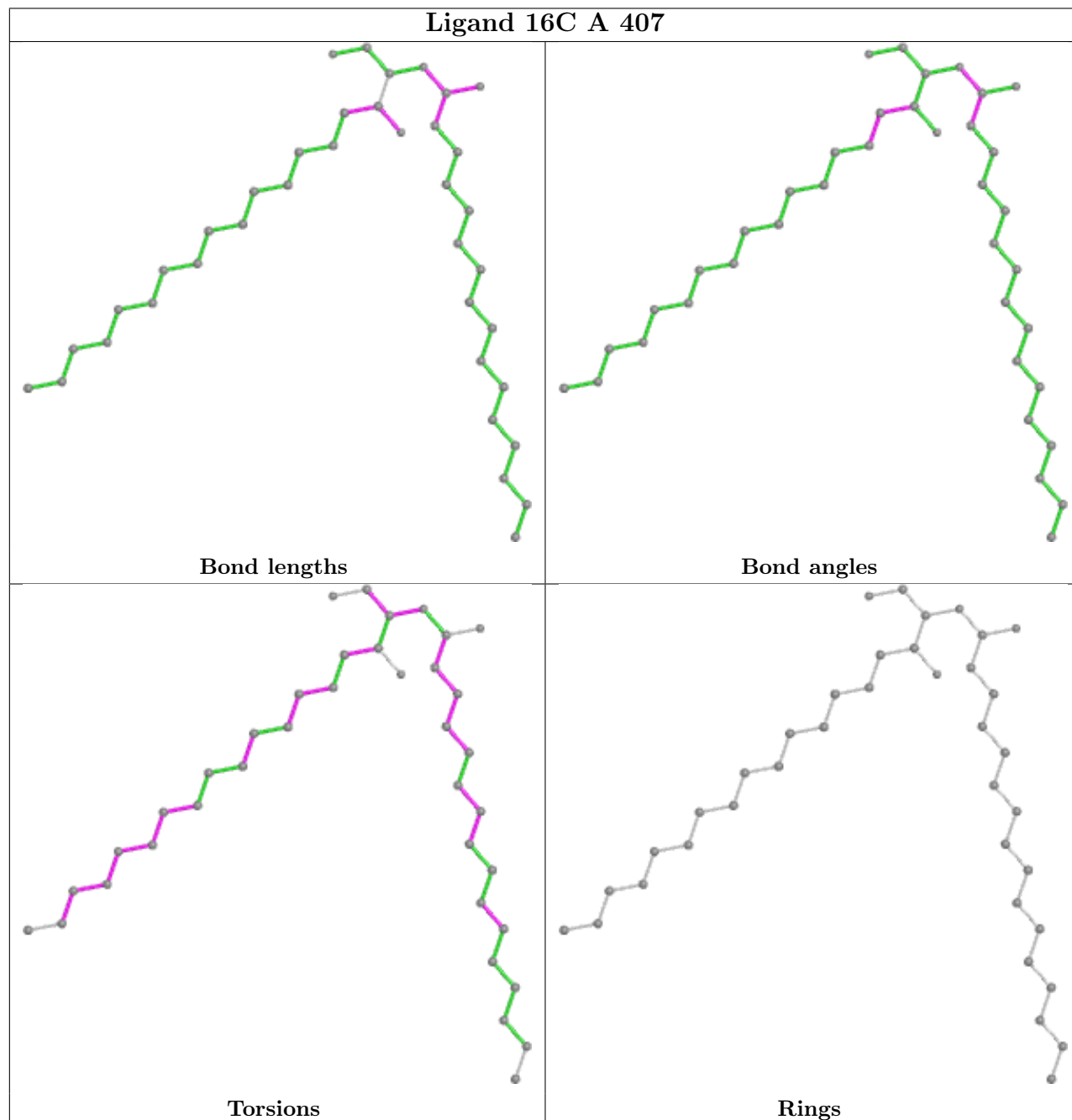
There are no ring outliers.

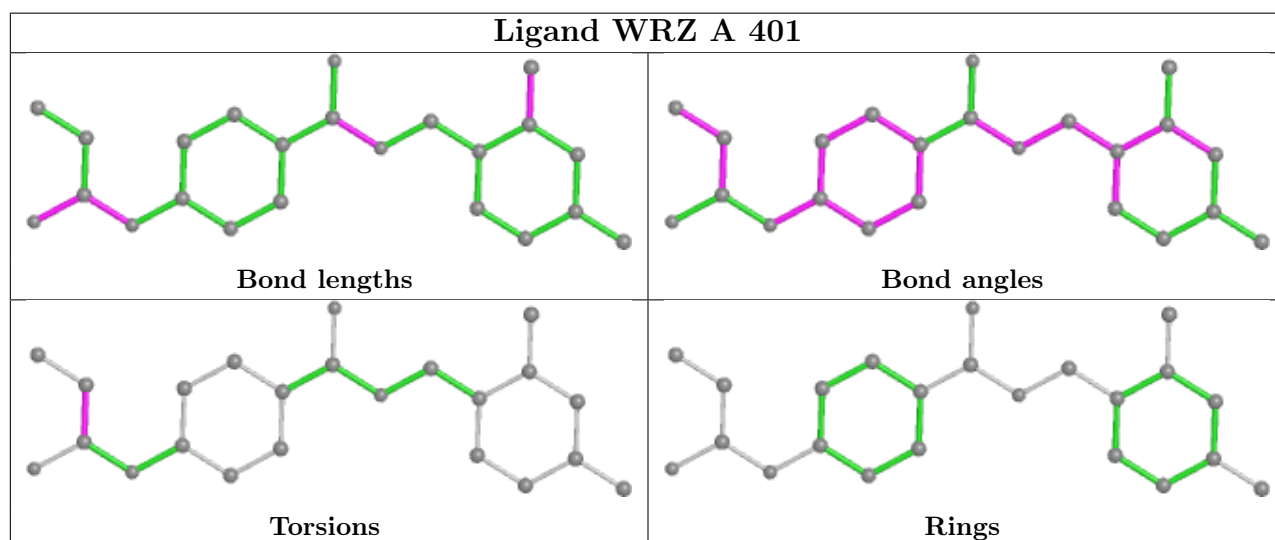
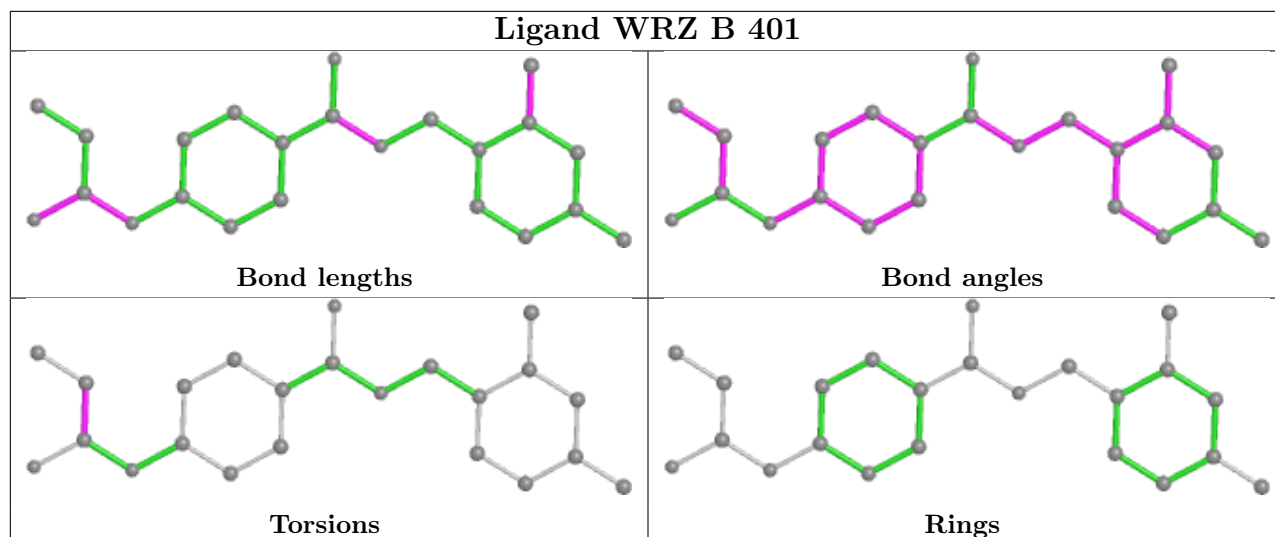
3 monomers are involved in 3 short contacts:

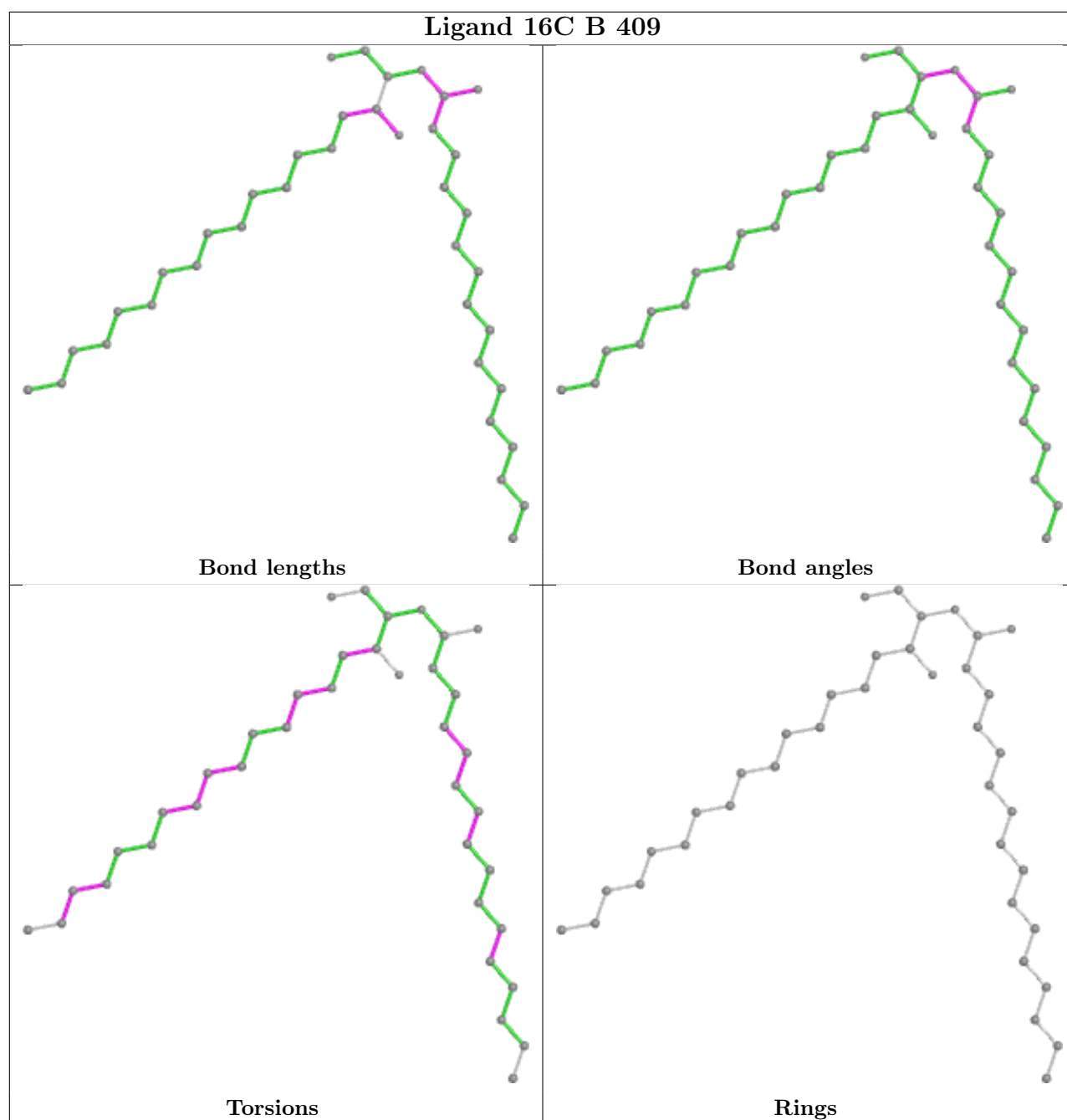
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	16C	1	0
2	B	401	WRZ	1	0
6	B	402	1PE	1	0

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	268/287 (93%)	0.56	36 (13%) <b>3</b>   <b>2</b>	62, 98, 187, 221	0
1	B	282/287 (98%)	0.58	38 (13%) <b>3</b>   <b>2</b>	62, 104, 196, 246	0
All	All	550/574 (95%)	0.57	74 (13%) <b>3</b>   <b>2</b>	62, 100, 195, 246	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	VAL	10.5
1	A	195	THR	9.1
1	A	315	ALA	8.5
1	B	95	SER	7.5
1	B	199	TRP	7.4
1	B	92	PRO	7.2
1	A	92	PRO	6.9
1	A	44	TRP	6.4
1	A	192	VAL	6.2
1	B	309	GLU	6.1
1	A	320	ASN	6.1
1	A	199	TRP	6.0
1	B	312	ALA	5.9
1	A	319	ALA	5.9
1	B	200	ASN	5.4
1	B	195	THR	5.4
1	A	200	ASN	5.3
1	B	93	CYS	4.8
1	B	203	GLN	4.8
1	A	316	GLU	4.7
1	B	113	GLY	4.3
1	B	196	PHE	3.9
1	A	196	PHE	3.9
1	A	191	LYS	3.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	86	LYS	3.8
1	A	194	ASP	3.8
1	A	112	ALA	3.8
1	B	207	ARG	3.7
1	A	98	GLU	3.5
1	B	316	GLU	3.5
1	A	321	VAL	3.4
1	B	122	ASN	3.3
1	B	35	SER	3.3
1	B	308	GLY	3.2
1	B	202	SER	3.1
1	A	232	HIS	3.1
1	B	36	ASP	3.0
1	A	198	LYS	3.0
1	A	318	THR	2.8
1	A	203	GLN	2.8
1	A	90	ALA	2.8
1	B	123	GLN	2.7
1	B	120	SER	2.7
1	B	104	GLN	2.7
1	A	193	GLU	2.6
1	A	263	ASP	2.6
1	B	205	LYS	2.6
1	A	202	SER	2.6
1	A	46	THR	2.5
1	A	268	ASP	2.5
1	A	127	TRP	2.5
1	B	115	ILE	2.5
1	A	206	ILE	2.5
1	B	111	ASN	2.4
1	B	311	ARG	2.4
1	A	81	VAL	2.4
1	A	307	VAL	2.4
1	B	89	ARG	2.4
1	B	96	ASP	2.4
1	A	89	ARG	2.4
1	B	65	PHE	2.3
1	B	197	ILE	2.3
1	B	313	HIS	2.3
1	B	204	THR	2.3
1	B	305	GLU	2.3
1	A	96	ASP	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	272	PRO	2.2
1	B	269	PHE	2.1
1	B	268	ASP	2.1
1	A	97	GLN	2.1
1	A	85	GLU	2.1
1	B	153	GLU	2.0
1	A	201	VAL	2.0
1	B	121	SER	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.

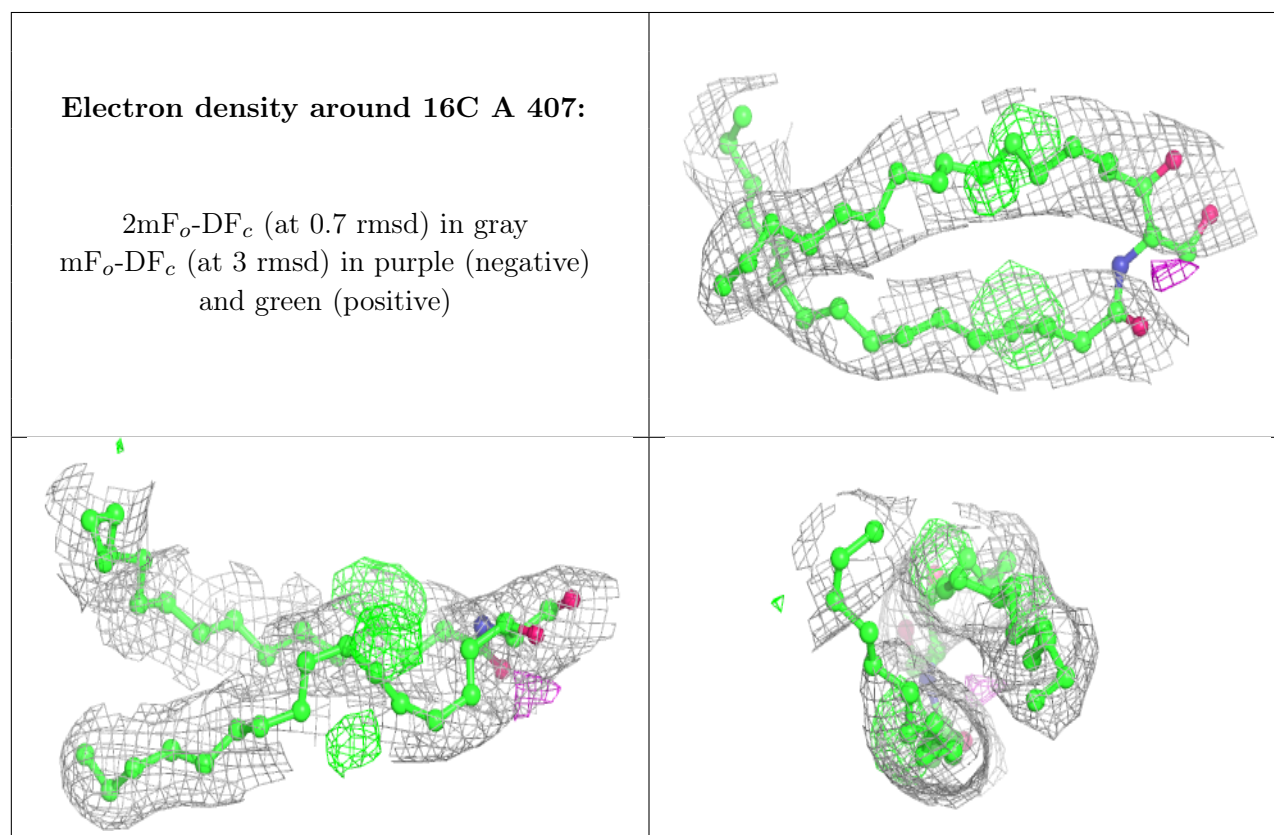
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	16C	A	407	38/38	0.64	0.28	78,106,143,159	0
3	D10	A	402	10/10	0.65	0.31	91,110,114,131	0
5	16C	B	409	38/38	0.70	0.20	73,110,144,148	0
8	D12	B	408	12/12	0.73	0.33	89,100,106,109	0
6	1PE	B	402	16/16	0.74	0.31	86,123,177,177	0
3	D10	A	403	10/10	0.80	0.24	87,106,116,117	0
7	CD	B	406	1/1	0.83	0.06	220,220,220,220	0
9	OCT	B	410	8/8	0.85	0.15	91,99,108,128	0
4	K	A	404	1/1	0.87	0.19	130,130,130,130	0
4	K	B	403	1/1	0.87	0.36	141,141,141,141	0
10	R16	B	412	16/16	0.87	0.17	76,84,99,102	0
9	OCT	B	411	8/8	0.90	0.31	90,97,109,115	0
2	WRZ	A	401	23/23	0.92	0.18	71,87,102,133	0
7	CD	B	407	1/1	0.92	0.12	132,132,132,132	0
2	WRZ	B	401	23/23	0.93	0.21	76,100,118,125	0

*Continued on next page...*

Continued from previous page...

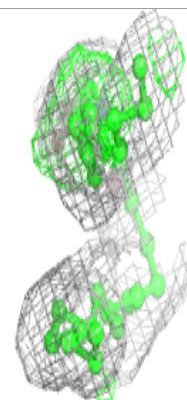
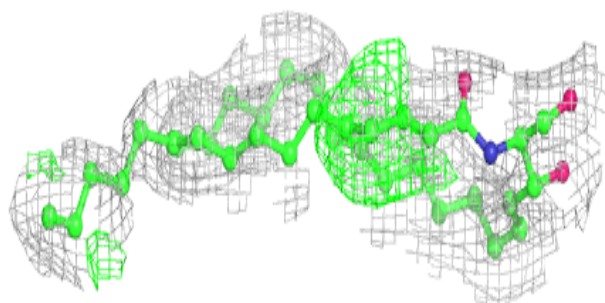
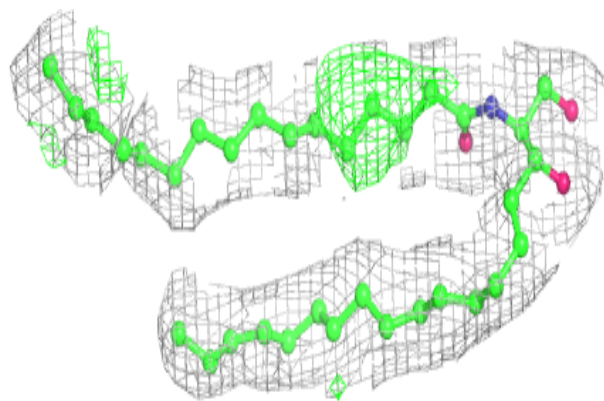
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	B	404	1/1	0.96	0.08	77,77,77,77	0
4	K	A	405	1/1	0.96	0.07	81,81,81,81	0
4	K	A	406	1/1	0.97	0.08	70,70,70,70	0
4	K	B	405	1/1	0.98	0.08	71,71,71,71	0

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.

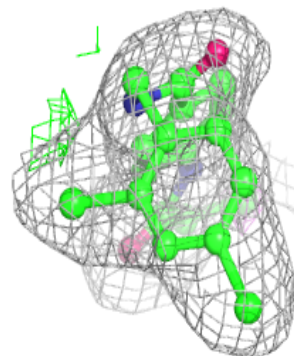
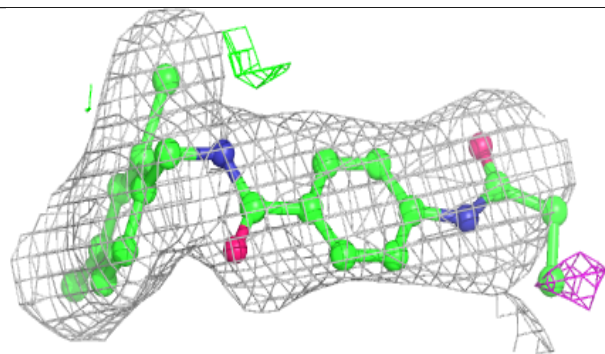
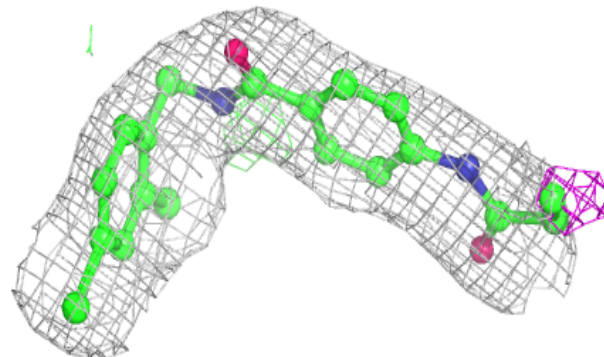


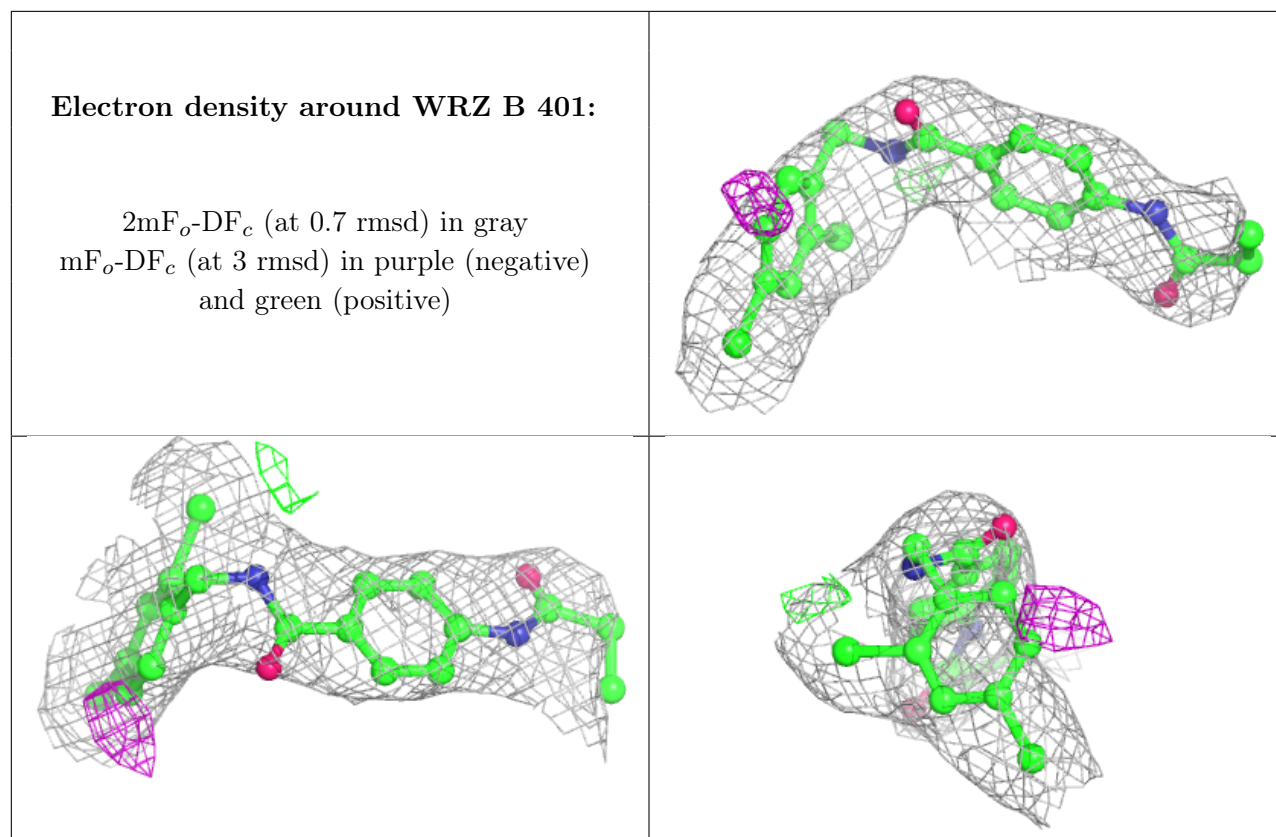
**Electron density around 16C B 409:**

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

**Electron density around WRZ A 401:**

$2mF_o-DF_c$  (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.