



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:22 PM JST

PDB ID : 7W1G  
Title : Crystal structure of YfiH with C107A mutation in complex with UDP-MurNAc-L-Serine  
Authors : Lee, S.H.; Hsieh, K.Y.; Lee, M.S.; Chang, C.I.  
Deposited on : 2021-11-19  
Resolution : 1.86 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

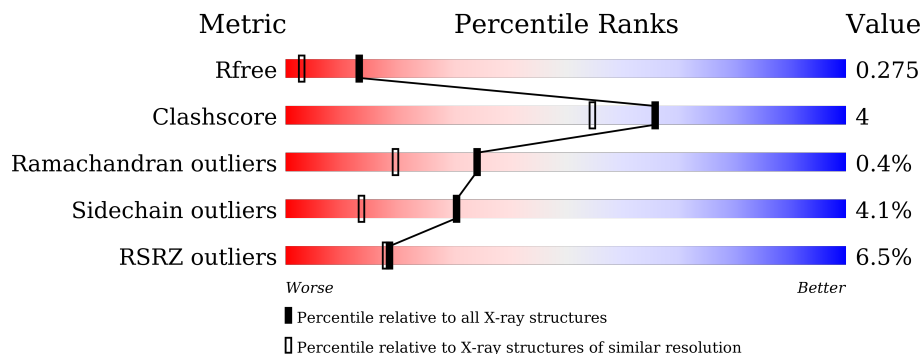
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	251	 4% (poor fit), 88% (0-1 outliers), 8% (2 outliers), 2% (3+ outliers), 2% (not modelled)
1	B	251	 6% (poor fit), 88% (0-1 outliers), 7% (2 outliers), 2% (3+ outliers), 2% (not modelled)
1	C	251	 8% (poor fit), 86% (0-1 outliers), 11% (2 outliers), 2% (3+ outliers), 2% (not modelled)
1	D	251	 8% (poor fit), 84% (0-1 outliers), 11% (2 outliers), 2% (3+ outliers), 2% (not modelled)

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8095 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 Purine nucleoside phosphorylase YfiH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1859	1173	330	346	10	0	2	0
1	B	242	1842	1163	326	343	10	0	0	0
1	C	243	1867	1179	331	347	10	0	2	0
1	D	243	1867	1179	332	346	10	0	2	0

There are 36 discrepancies between the modelled and reference sequences:

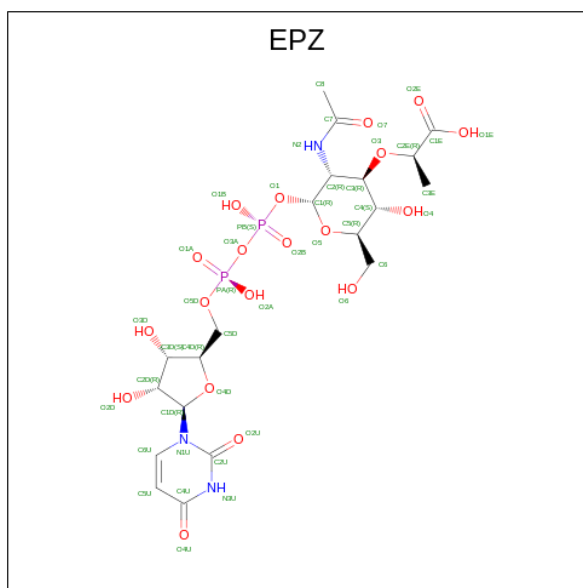
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	CYS	engineered mutation	UNP P33644
A	244	LEU	-	expression tag	UNP P33644
A	245	GLU	-	expression tag	UNP P33644
A	246	HIS	-	expression tag	UNP P33644
A	247	HIS	-	expression tag	UNP P33644
A	248	HIS	-	expression tag	UNP P33644
A	249	HIS	-	expression tag	UNP P33644
A	250	HIS	-	expression tag	UNP P33644
A	251	HIS	-	expression tag	UNP P33644
B	107	ALA	CYS	engineered mutation	UNP P33644
B	244	LEU	-	expression tag	UNP P33644
B	245	GLU	-	expression tag	UNP P33644
B	246	HIS	-	expression tag	UNP P33644
B	247	HIS	-	expression tag	UNP P33644
B	248	HIS	-	expression tag	UNP P33644
B	249	HIS	-	expression tag	UNP P33644
B	250	HIS	-	expression tag	UNP P33644
B	251	HIS	-	expression tag	UNP P33644
C	107	ALA	CYS	engineered mutation	UNP P33644
C	244	LEU	-	expression tag	UNP P33644
C	245	GLU	-	expression tag	UNP P33644

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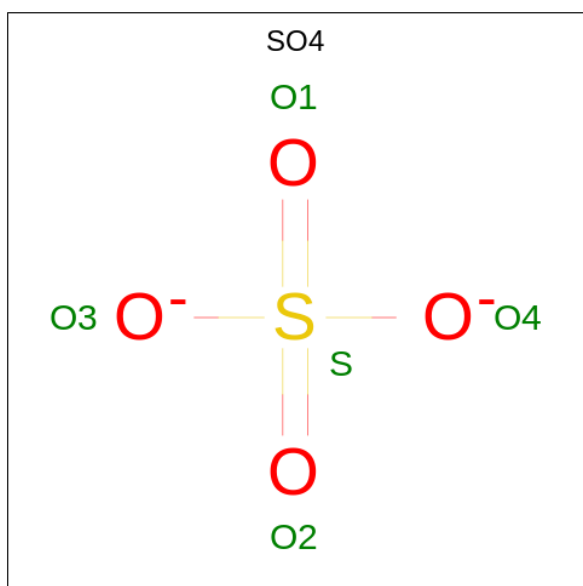
Chain	Residue	Modelled	Actual	Comment	Reference
C	246	HIS	-	expression tag	UNP P33644
C	247	HIS	-	expression tag	UNP P33644
C	248	HIS	-	expression tag	UNP P33644
C	249	HIS	-	expression tag	UNP P33644
C	250	HIS	-	expression tag	UNP P33644
C	251	HIS	-	expression tag	UNP P33644
D	107	ALA	CYS	engineered mutation	UNP P33644
D	244	LEU	-	expression tag	UNP P33644
D	245	GLU	-	expression tag	UNP P33644
D	246	HIS	-	expression tag	UNP P33644
D	247	HIS	-	expression tag	UNP P33644
D	248	HIS	-	expression tag	UNP P33644
D	249	HIS	-	expression tag	UNP P33644
D	250	HIS	-	expression tag	UNP P33644
D	251	HIS	-	expression tag	UNP P33644

- Molecule 2 is (2R)-2-[[[(2R,3R,4R,5S,6R)-3-(acetylamino)-2-[[[(S)-[[[(R)-[[[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-5-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4-yl]oxy}propanoic acid (three-letter code: EPZ) (formula: C<sub>20</sub>H<sub>31</sub>N<sub>3</sub>O<sub>19</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



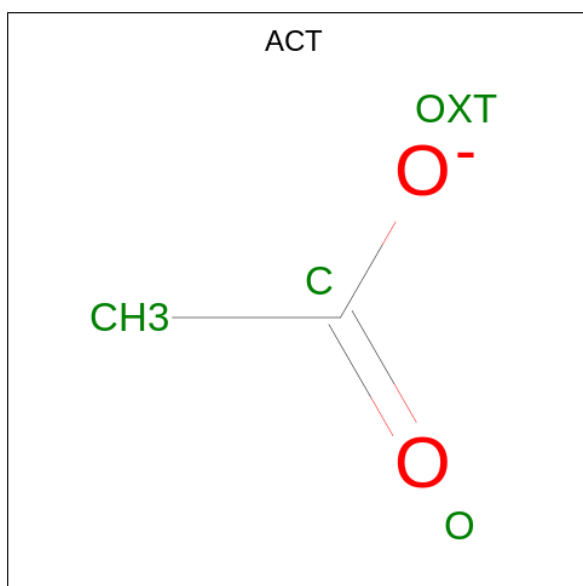
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



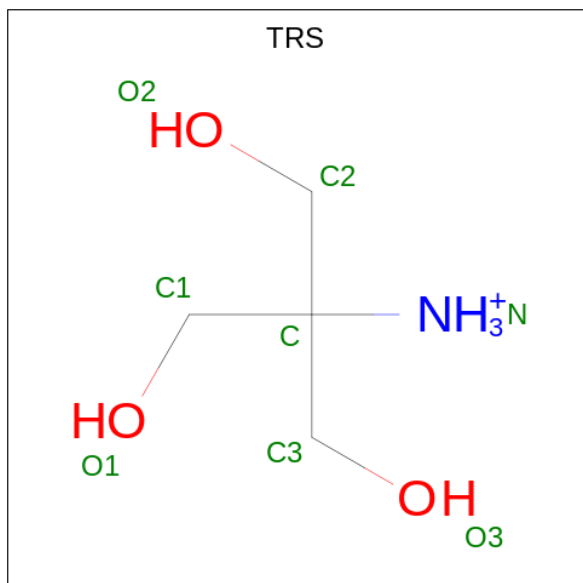
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0

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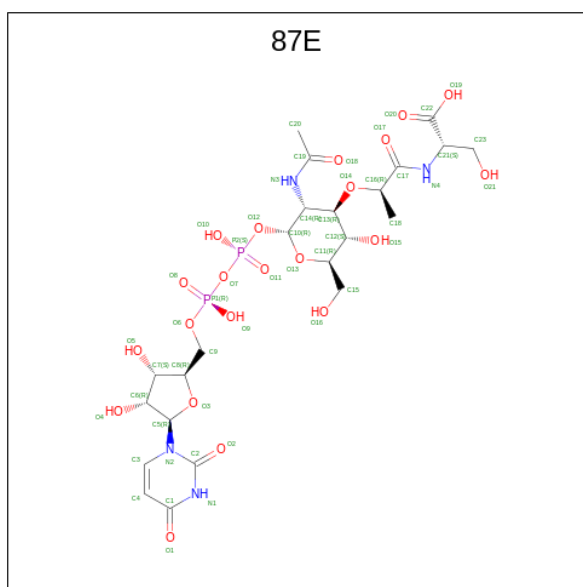
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is (2S)-2-[[[(2R)-2-[(2R,3R,4R,5S,6R)-3-acetamido-2-[[[(2R,3S,4R,5R)-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-6-(hydroxymethyl)-5-oxidanyl-oxan-4-yl]oxypropanoyl]amino]-3-oxidanyl-propanoic acid (three-letter code: 87E) (formula: C<sub>23</sub>H<sub>36</sub>N<sub>4</sub>O<sub>21</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
6	C	1	50	23	4	21	2	0	0
6	D	1	50	23	4	21	2	0	0

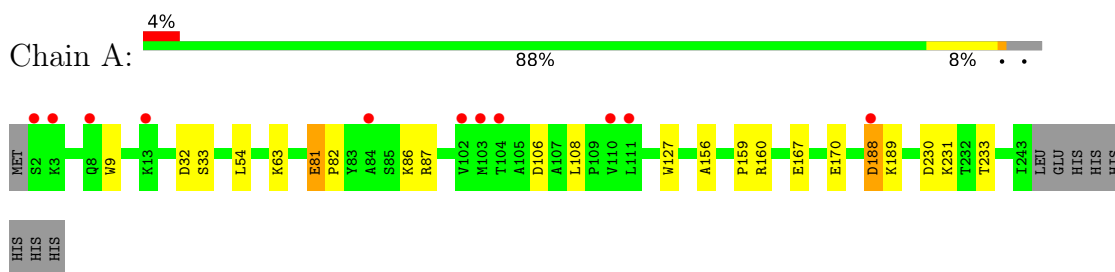
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	B	124	Total	O	0	0
			124	124		
7	C	83	Total	O	0	0
			83	83		
7	D	97	Total	O	0	0
			97	97		

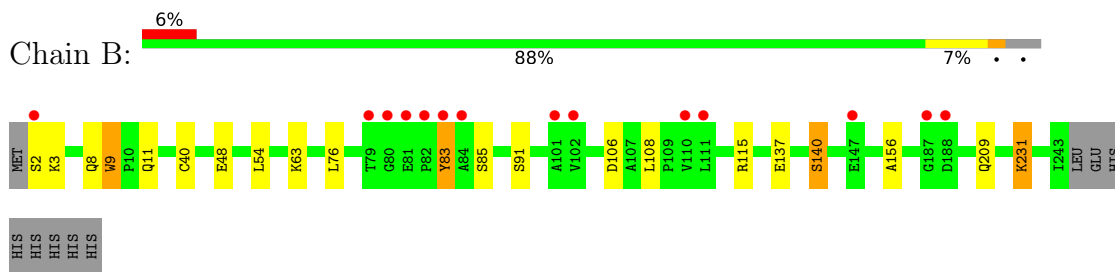
### 3 Residue-property plots [i](#)

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.

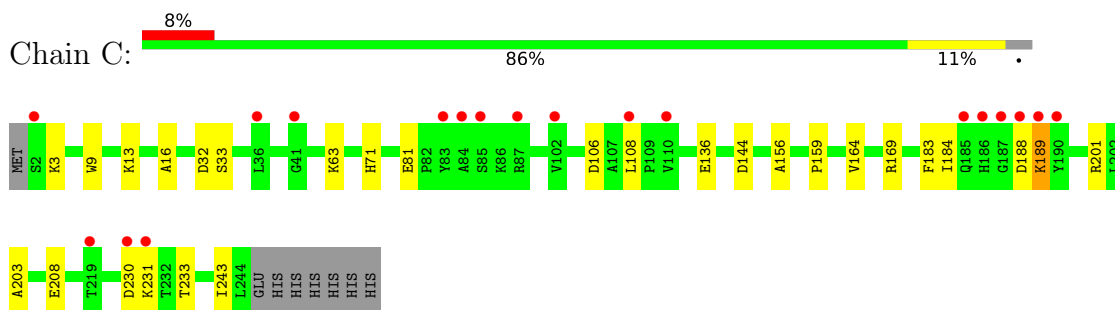
- Molecule 1: Purine nucleoside phosphorylase YfiH



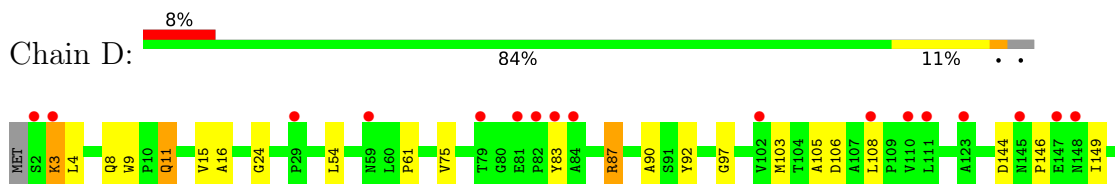
- Molecule 1: Purine nucleoside phosphorylase YfiH



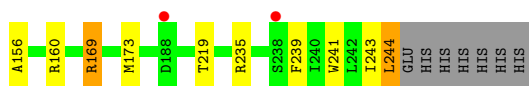
- Molecule 1: Purine nucleoside phosphorylase YfiH



- Molecule 1: Purine nucleoside phosphorylase YfiH







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.56Å 99.24Å 136.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.45 – 1.86 27.44 – 1.86	Depositor EDS
% Data completeness (in resolution range)	92.3 (27.45-1.86) 92.4 (27.44-1.86)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.215 , 0.266 0.227 , 0.275	Depositor DCC
$R_{free}$ test set	3699 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: SO4, TRS, 87E, EPZ, ACT

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	0.72	0/1907	0.86	0/2593
1	B	0.71	0/1887	0.84	0/2566
1	C	0.71	0/1915	0.80	0/2603
1	D	0.70	0/1915	0.85	2/2603 (0.1%)
All	All	0.71	0/7624	0.84	2/10365 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	D	169	ARG	NE-CZ-NH2	-6.37	117.12	120.30

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	1859	0	1815	17	0
1	B	1842	0	1797	14	0
1	C	1867	0	1826	14	0
1	D	1867	0	1828	22	0
2	A	44	0	28	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	28	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
5	B	8	0	12	2	0
6	C	50	0	0	2	0
6	D	50	0	0	1	0
7	A	138	0	0	4	0
7	B	124	0	0	1	0
7	C	83	0	0	0	0
7	D	97	0	0	3	0
All	All	8095	0	7343	60	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 4.

All (60) 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:127:TRP:H	2:A:301:EPZ:H8	1.39	0.88
1:C:208[B]:GLU:HB3	1:D:219:THR:HG22	1.76	0.68
1:C:203:ALA:O	1:D:160:ARG:NH2	2.25	0.67
1:A:127:TRP:CD1	2:A:301:EPZ:H8B	2.34	0.63
1:A:127:TRP:H	2:A:301:EPZ:C8	2.12	0.62
1:D:103:MET:HG3	7:D:423:HOH:O	1.98	0.62
1:C:230:ASP:HB2	1:C:233:THR:HB	1.85	0.58
1:D:4:LEU:HD21	1:D:54:LEU:HD21	1.85	0.58
1:D:146:PRO:HA	1:D:149:ILE:HD12	1.87	0.57
1:A:160:ARG:NH1	1:B:9:TRP:O	2.38	0.56
1:B:137:GLU:O	1:B:140:SER:HB2	2.05	0.56
1:A:127:TRP:N	2:A:301:EPZ:H8	2.18	0.54
1:A:54:LEU:C	1:A:54:LEU:HD13	2.28	0.54
1:D:87:ARG:NH1	7:D:403:HOH:O	2.40	0.54
1:D:97:GLY:CA	1:D:244:LEU:HD23	2.38	0.53
1:A:81[A]:GLU:HG2	1:A:82:PRO:HA	1.91	0.53
7:A:472:HOH:O	1:C:63:LYS:HG3	2.09	0.53
1:D:11:GLN:OE1	1:D:15:VAL:O	2.26	0.53
1:D:97:GLY:HA3	1:D:244:LEU:HD23	1.91	0.53
1:C:16:ALA:HB2	1:C:243:ILE:HD11	1.90	0.53
1:A:160:ARG:NH1	1:B:11:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:HE3	1:B:231:LYS:HA	1.92	0.51
1:B:209:GLN:NE2	7:B:403:HOH:O	2.40	0.50
1:B:108:LEU:HA	1:B:156:ALA:HB2	1.93	0.50
1:D:108:LEU:HA	1:D:156:ALA:HB2	1.95	0.49
1:D:169:ARG:NH1	1:D:173:MET:SD	2.86	0.48
1:D:75:VAL:HG22	1:D:90:ALA:HB3	1.95	0.48
1:B:115:ARG:NH2	1:B:209:GLN:OE1	2.47	0.48
1:A:87:ARG:NH2	7:A:403:HOH:O	2.40	0.48
1:D:3:LYS:HG2	1:D:24:GLY:HA3	1.95	0.47
1:D:54:LEU:HD11	1:D:239:PHE:CE1	2.50	0.46
1:A:108:LEU:HA	1:A:156:ALA:HB2	1.96	0.46
1:D:4:LEU:HD21	1:D:54:LEU:CD2	2.45	0.46
1:A:127:TRP:HD1	2:A:301:EPZ:H8B	1.78	0.46
1:C:108:LEU:HA	1:C:156:ALA:HB2	1.98	0.46
1:C:32:ASP:HA	1:C:33:SER:HA	1.63	0.46
1:A:189:LYS:NZ	7:A:413:HOH:O	2.49	0.45
1:B:76:LEU:O	1:B:91:SER:HA	2.16	0.45
1:A:32:ASP:HA	1:A:33:SER:HA	1.75	0.44
1:D:235:ARG:HE	6:D:301:87E:C22	2.29	0.44
1:A:86:LYS:NZ	7:A:415:HOH:O	2.50	0.44
1:A:188:ASP:N	1:A:188:ASP:OD1	2.50	0.44
1:C:71:HIS:NE2	6:C:301:87E:C23	2.81	0.44
1:C:189:LYS:HD2	1:C:189:LYS:N	2.33	0.43
1:A:230:ASP:HB2	1:A:233:THR:HB	2.00	0.43
1:C:164:VAL:HA	6:C:301:87E:O3	2.18	0.43
1:B:48:GLU:HG3	5:B:304:TRS:H11	2.00	0.42
1:D:105:ALA:HB2	1:D:235:ARG:HD3	2.02	0.41
1:C:136:GLU:OE2	1:C:201:ARG:HD2	2.19	0.41
1:B:83:TYR:CD1	1:B:83:TYR:N	2.87	0.41
1:B:2:SER:OG	1:B:3:LYS:N	2.53	0.41
1:C:208[B]:GLU:HB3	1:D:219:THR:CG2	2.47	0.41
1:D:4:LEU:HD23	1:D:4:LEU:HA	1.93	0.41
1:D:16:ALA:HA	7:D:427:HOH:O	2.20	0.41
1:B:54:LEU:C	1:B:54:LEU:HD13	2.40	0.41
1:D:61:PRO:HD3	1:D:241:TRP:NE1	2.36	0.41
1:A:159:PRO:HG2	1:B:8:GLN:HB3	2.02	0.41
1:C:159:PRO:HG2	1:D:8[B]:GLN:HB3	2.01	0.40
1:B:63:LYS:HE3	5:B:304:TRS:H32	2.04	0.40
1:C:183:PHE:C	1:C:184:ILE:HD12	2.42	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	242/251 (96%)	233 (96%)	8 (3%)	1 (0%)	34	19
1	B	240/251 (96%)	231 (96%)	8 (3%)	1 (0%)	34	19
1	C	243/251 (97%)	234 (96%)	8 (3%)	1 (0%)	34	19
1	D	243/251 (97%)	228 (94%)	14 (6%)	1 (0%)	34	19
All	All	968/1004 (96%)	926 (96%)	38 (4%)	4 (0%)	34	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	B	106	ASP
1	C	106	ASP
1	D	106	ASP

### 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	191/198 (96%)	183 (96%)	8 (4%)	30	13
1	B	189/198 (96%)	183 (97%)	6 (3%)	39	22
1	C	192/198 (97%)	183 (95%)	9 (5%)	26	10
1	D	192/198 (97%)	183 (95%)	9 (5%)	26	10
All	All	764/792 (96%)	732 (96%)	32 (4%)	30	13

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	63	LYS
1	A	81[A]	GLU
1	A	81[B]	GLU
1	A	167	GLU
1	A	170	GLU
1	A	188	ASP
1	A	231	LYS
1	B	9	TRP
1	B	40	CYS
1	B	83	TYR
1	B	85	SER
1	B	140	SER
1	B	231	LYS
1	C	3	LYS
1	C	9	TRP
1	C	13	LYS
1	C	81	GLU
1	C	144	ASP
1	C	169	ARG
1	C	188	ASP
1	C	189	LYS
1	C	231	LYS
1	D	3	LYS
1	D	9	TRP
1	D	11	GLN
1	D	83	TYR
1	D	87	ARG
1	D	92	TYR
1	D	144	ASP
1	D	243	ILE
1	D	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	209	GLN
1	D	209	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	SO4	B	305	-	4,4,4	0.29	0	6,6,6	0.13	0
2	EPZ	A	301	-	43,46,46	0.53	0	60,69,69	0.69	1 (1%)
6	87E	D	301	-	49,52,52	3.20	25 (51%)	68,77,77	1.66	13 (19%)
6	87E	C	301	-	49,52,52	3.18	21 (42%)	68,77,77	1.94	17 (25%)
3	SO4	A	302	-	4,4,4	0.36	0	6,6,6	0.12	0
2	EPZ	B	301	-	43,46,46	0.50	0	60,69,69	0.72	1 (1%)
4	ACT	C	302	-	3,3,3	1.00	0	3,3,3	0.82	0
5	TRS	B	304	-	7,7,7	0.18	0	9,9,9	0.70	0
4	ACT	B	302	-	3,3,3	0.92	0	3,3,3	0.91	0
4	ACT	B	303	-	3,3,3	1.12	0	3,3,3	0.64	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
2	EPZ	A	301	-	-	8/34/71/71	0/3/3/3
6	87E	C	301	-	-	7/44/81/81	0/3/3/3
2	EPZ	B	301	-	-	3/34/71/71	0/3/3/3
5	TRS	B	304	-	-	6/9/9/9	-
6	87E	D	301	-	-	6/44/81/81	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	87E	O2-C2	11.18	1.43	1.23
6	D	301	87E	O2-C2	10.55	1.42	1.23
6	D	301	87E	C7-C6	-10.48	1.24	1.53
6	C	301	87E	C7-C6	-10.00	1.26	1.53
6	C	301	87E	C17-N4	6.43	1.48	1.34
6	D	301	87E	C17-N4	5.66	1.46	1.34
6	C	301	87E	C14-N3	5.51	1.54	1.45
6	D	301	87E	O3-C5	-4.70	1.30	1.42
6	D	301	87E	C14-N3	4.43	1.52	1.45
6	C	301	87E	O13-C10	4.31	1.52	1.41
6	C	301	87E	C6-C5	4.28	1.67	1.53
6	D	301	87E	C6-C5	4.06	1.66	1.53
6	D	301	87E	C19-N3	3.73	1.47	1.34
6	C	301	87E	C7-C8	3.60	1.62	1.53
6	C	301	87E	C19-N3	3.57	1.46	1.34
6	D	301	87E	C9-C8	-3.53	1.40	1.51
6	C	301	87E	O5-C7	3.48	1.51	1.43
6	D	301	87E	C13-C14	-3.44	1.47	1.53
6	C	301	87E	O3-C5	-3.42	1.33	1.42
6	D	301	87E	O17-C17	-3.39	1.16	1.23
6	C	301	87E	O14-C16	-3.24	1.37	1.44
6	D	301	87E	O13-C10	3.16	1.49	1.41
6	D	301	87E	O1-C1	-3.15	1.18	1.24
6	D	301	87E	C2-N1	-3.15	1.32	1.38
6	C	301	87E	C9-C8	-3.10	1.41	1.51
6	C	301	87E	C20-C19	3.10	1.57	1.50
6	D	301	87E	O5-C7	3.09	1.50	1.43
6	D	301	87E	O14-C16	-2.99	1.37	1.44
6	D	301	87E	C2-N2	-2.94	1.33	1.38
6	C	301	87E	O17-C17	-2.92	1.17	1.23
6	D	301	87E	C1-N1	-2.92	1.33	1.38
6	C	301	87E	O1-C1	-2.91	1.18	1.24
6	C	301	87E	O3-C8	2.90	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	87E	O3-C8	2.87	1.51	1.45
6	D	301	87E	C20-C19	2.82	1.56	1.50
6	D	301	87E	C7-C8	2.67	1.59	1.53
6	C	301	87E	C13-C14	-2.66	1.48	1.53
6	D	301	87E	C4-C1	-2.46	1.38	1.43
6	D	301	87E	P1-O9	-2.38	1.44	1.55
6	C	301	87E	P1-O6	2.37	1.68	1.59
6	D	301	87E	P2-O12	2.29	1.66	1.60
6	C	301	87E	O4-C6	2.27	1.48	1.43
6	C	301	87E	C2-N1	-2.21	1.34	1.38
6	C	301	87E	C3-C4	2.14	1.40	1.35
6	D	301	87E	P2-O10	-2.13	1.45	1.55
6	D	301	87E	P1-O8	-2.07	1.43	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	87E	C18-C16-C17	-5.13	98.43	111.11
6	C	301	87E	C21-N4-C17	4.52	131.36	121.67
6	D	301	87E	N1-C2-N2	4.46	120.81	114.89
6	C	301	87E	C1-N1-C2	-4.46	120.70	126.58
6	C	301	87E	N1-C2-N2	4.27	120.56	114.89
6	D	301	87E	C1-N1-C2	-4.06	121.22	126.58
6	C	301	87E	C4-C1-N1	4.05	120.90	114.84
6	C	301	87E	O17-C17-N4	4.05	130.43	122.93
6	C	301	87E	C10-C14-N3	-3.68	104.67	111.00
6	D	301	87E	O7-P2-O12	3.45	109.44	102.48
6	D	301	87E	P2-O7-P1	-3.40	121.16	132.83
6	C	301	87E	P2-O7-P1	-3.39	121.18	132.83
6	C	301	87E	O1-C1-C4	-3.37	119.23	125.16
6	D	301	87E	C4-C1-N1	3.36	119.86	114.84
6	D	301	87E	O1-C1-C4	-3.10	119.70	125.16
6	C	301	87E	O14-C16-C17	-3.08	104.54	111.17
6	D	301	87E	C18-C16-C17	-3.05	103.57	111.11
6	D	301	87E	C10-C14-N3	-2.79	106.20	111.00
6	C	301	87E	O2-C2-N1	-2.70	116.46	121.50
6	C	301	87E	C5-N2-C2	2.47	122.04	117.57
6	D	301	87E	C21-N4-C17	2.30	126.60	121.67
2	A	301	EPZ	C3-C2-N2	2.29	114.71	110.91
6	D	301	87E	C15-C11-C12	-2.28	107.67	113.00
6	D	301	87E	O13-C11-C12	2.24	113.77	109.69
6	C	301	87E	O5-C7-C8	-2.24	104.59	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	87E	O18-C19-N3	-2.22	117.87	121.95
2	B	301	EPZ	O5-C1-O1	-2.09	108.63	111.36
6	C	301	87E	O12-C10-C14	-2.08	104.64	108.40
6	C	301	87E	O7-P2-O12	2.06	106.65	102.48
6	C	301	87E	C16-C17-N4	-2.04	111.86	118.28
6	D	301	87E	O5-C7-C8	-2.04	105.15	111.05
6	D	301	87E	C4-C3-N2	-2.01	118.44	121.81

There are no chirality outliers.

All (30) torsion outliers are listed below:

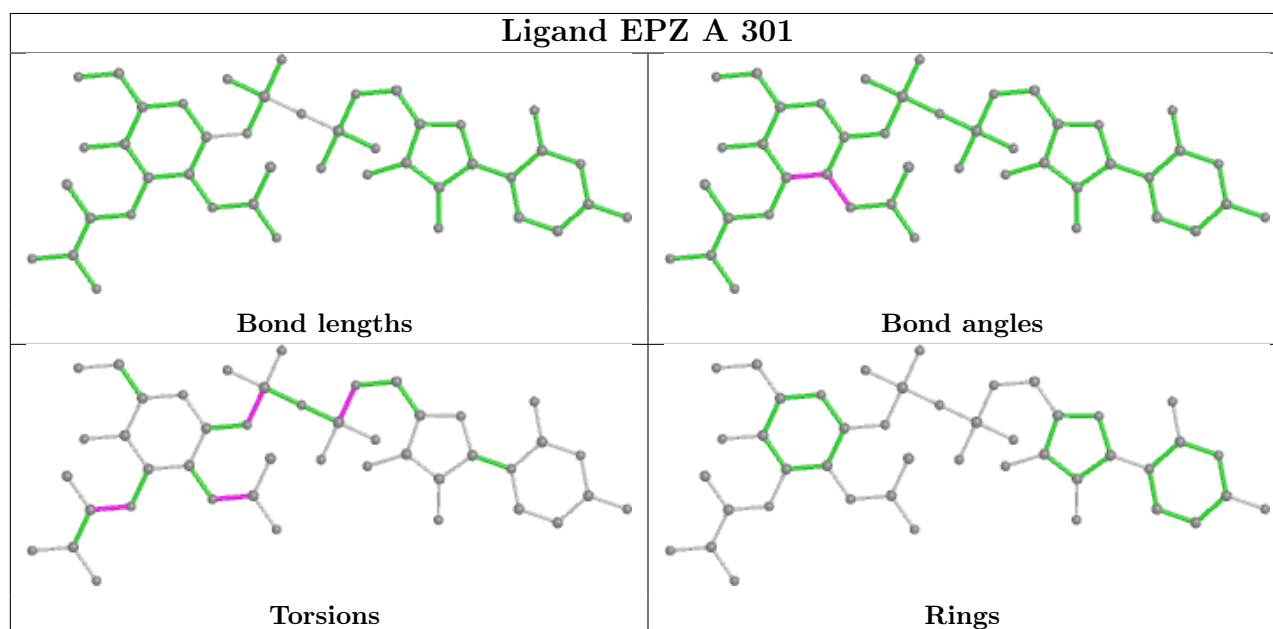
Mol	Chain	Res	Type	Atoms
2	A	301	EPZ	C5D-O5D-PA-O1A
2	B	301	EPZ	C5D-O5D-PA-O1A
5	B	304	TRS	C1-C-C3-O3
5	B	304	TRS	C2-C-C3-O3
5	B	304	TRS	N-C-C3-O3
6	C	301	87E	C9-O6-P1-O8
6	C	301	87E	C9-O6-P1-O9
6	C	301	87E	N4-C21-C23-O21
6	D	301	87E	C9-O6-P1-O8
6	D	301	87E	C9-O6-P1-O9
6	D	301	87E	C18-C16-O14-C13
2	A	301	EPZ	O7-C7-N2-C2
2	A	301	EPZ	C8-C7-N2-C2
6	D	301	87E	C12-C11-C15-O16
6	C	301	87E	C22-C21-C23-O21
6	C	301	87E	N4-C21-C22-O20
6	C	301	87E	N4-C21-C22-O19
2	A	301	EPZ	C5D-O5D-PA-O3A
2	B	301	EPZ	C5D-O5D-PA-O3A
6	D	301	87E	C9-O6-P1-O7
5	B	304	TRS	N-C-C1-O1
2	B	301	EPZ	C5D-O5D-PA-O2A
2	A	301	EPZ	C1-O1-PB-O3A
6	D	301	87E	P1-O7-P2-O11
2	A	301	EPZ	C1-O1-PB-O1B
5	B	304	TRS	C2-C-C1-O1
6	C	301	87E	C9-O6-P1-O7
5	B	304	TRS	C3-C-C1-O1
2	A	301	EPZ	C5D-O5D-PA-O2A
2	A	301	EPZ	C3E-C2E-O3-C3

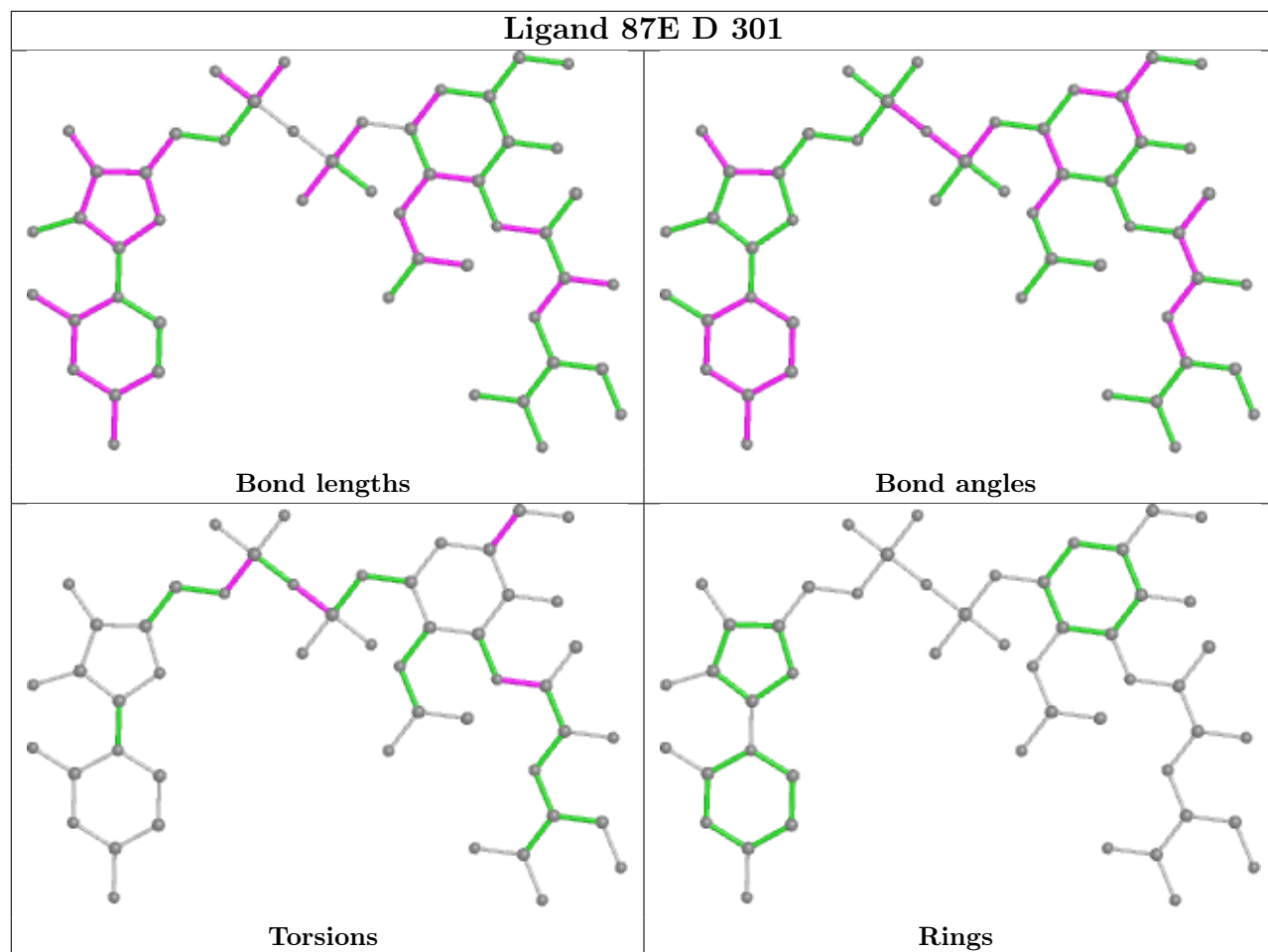
There are no ring outliers.

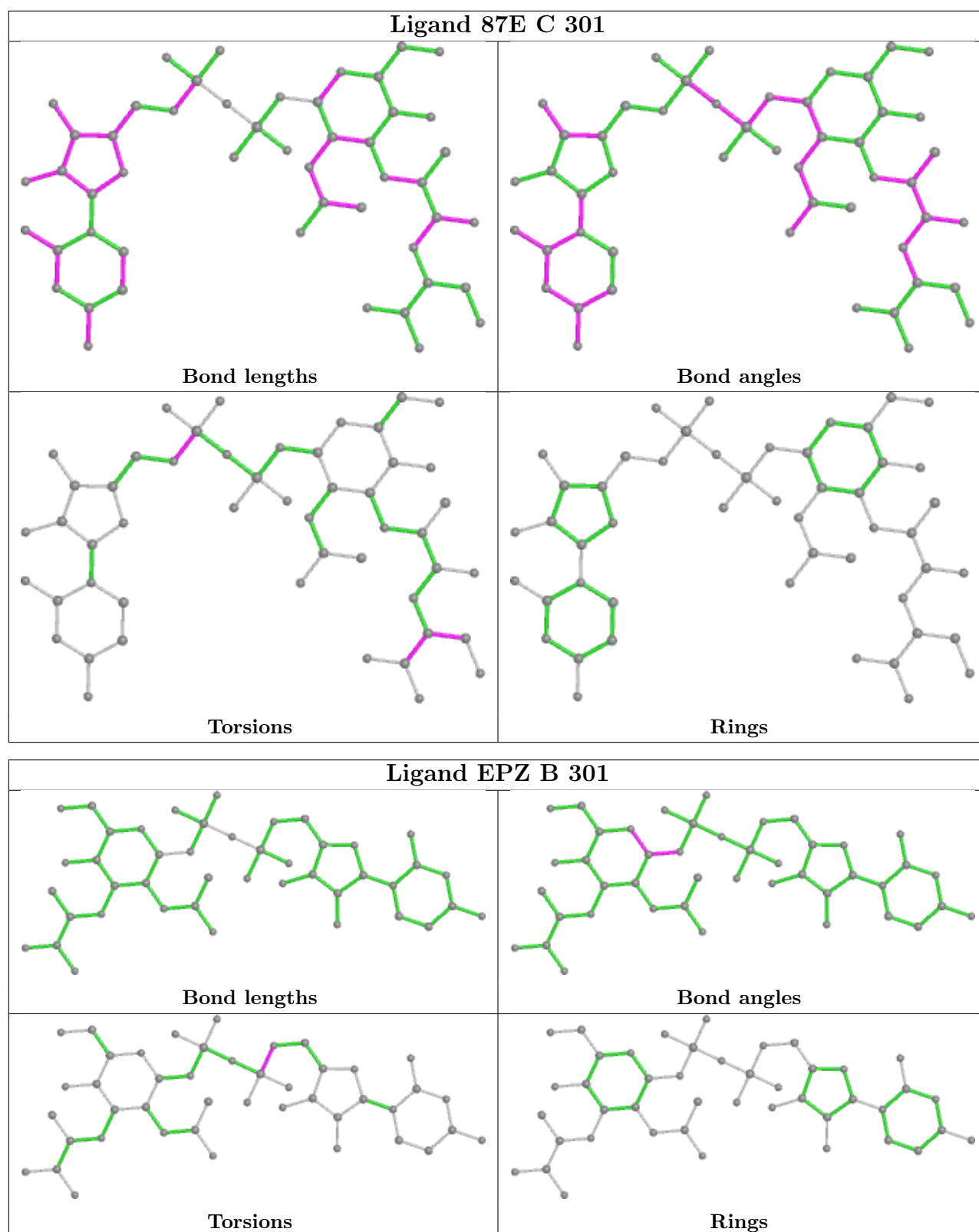
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EPZ	5	0
6	D	301	87E	1	0
6	C	301	87E	2	0
5	B	304	TRS	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 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

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	242/251 (96%)	0.11	11 (4%) 33 32	20, 28, 44, 70	0
1	B	242/251 (96%)	0.30	14 (5%) 23 22	22, 30, 49, 102	0
1	C	243/251 (96%)	0.33	19 (7%) 13 13	22, 32, 54, 87	0
1	D	243/251 (96%)	0.44	19 (7%) 13 13	25, 35, 55, 86	0
All	All	970/1004 (96%)	0.29	63 (6%) 18 18	20, 31, 51, 102	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	PRO	8.3
1	C	84	ALA	5.2
1	B	81	GLU	5.2
1	C	2	SER	5.2
1	B	83	TYR	5.1
1	D	82	PRO	5.1
1	B	84	ALA	4.4
1	D	84	ALA	4.4
1	C	187	GLY	4.1
1	B	2	SER	3.7
1	D	102	VAL	3.6
1	B	110	VAL	3.5
1	D	108	LEU	3.5
1	D	2	SER	3.4
1	D	79	THR	3.3
1	C	188	ASP	3.3
1	A	2	SER	3.2
1	A	102	VAL	3.1
1	D	59	ASN	3.1
1	A	13	LYS	3.0
1	B	102	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	145	ASN	3.0
1	C	185	GLN	2.8
1	C	41	GLY	2.8
1	D	110	VAL	2.8
1	D	111	LEU	2.8
1	B	79	THR	2.8
1	B	111	LEU	2.7
1	D	123	ALA	2.6
1	C	186	HIS	2.6
1	C	219	THR	2.6
1	A	188	ASP	2.5
1	B	101	ALA	2.5
1	C	230	ASP	2.5
1	C	102	VAL	2.4
1	A	8	GLN	2.4
1	D	238	SER	2.4
1	C	87	ARG	2.4
1	B	188	ASP	2.3
1	D	29	PRO	2.3
1	D	3	LYS	2.3
1	B	80	GLY	2.3
1	C	36	LEU	2.3
1	A	110	VAL	2.3
1	D	188	ASP	2.3
1	A	111	LEU	2.3
1	D	83	TYR	2.3
1	C	231	LYS	2.3
1	A	84	ALA	2.3
1	B	147	GLU	2.3
1	B	187	GLY	2.2
1	C	190	TYR	2.2
1	C	85	SER	2.2
1	D	81	GLU	2.2
1	A	104	THR	2.1
1	C	83	TYR	2.1
1	D	147	GLU	2.1
1	D	148	ASN	2.1
1	A	103	MET	2.1
1	A	3	LYS	2.1
1	C	108	LEU	2.1
1	C	110	VAL	2.0
1	C	189	LYS	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](#)

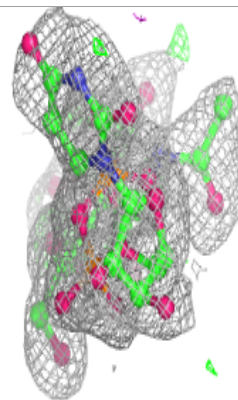
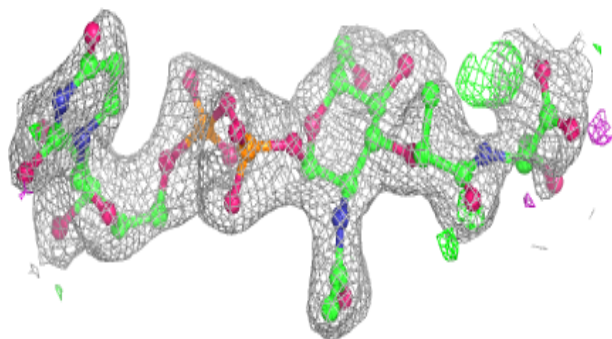
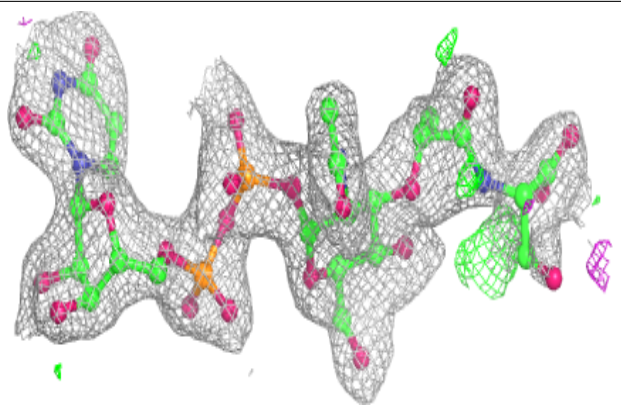
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	TRS	B	304	8/8	0.72	0.27	50,52,58,66	0
4	ACT	B	302	4/4	0.87	0.12	37,39,42,47	0
6	87E	C	301	50/50	0.87	0.16	37,48,65,72	0
4	ACT	B	303	4/4	0.92	0.12	35,38,40,40	0
2	EPZ	A	301	44/44	0.93	0.11	22,34,40,48	0
3	SO4	A	302	5/5	0.94	0.11	53,54,60,61	0
6	87E	D	301	50/50	0.94	0.12	23,29,60,64	0
4	ACT	C	302	4/4	0.95	0.09	49,49,51,52	0
2	EPZ	B	301	44/44	0.96	0.09	23,28,32,34	0
3	SO4	B	305	5/5	0.96	0.10	46,49,53,57	0

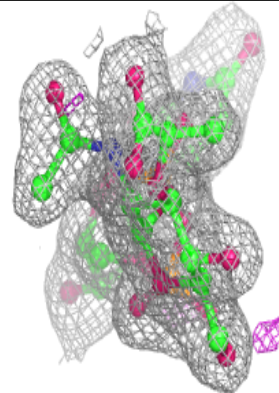
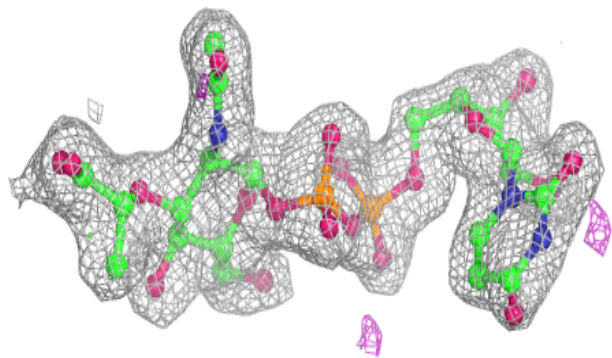
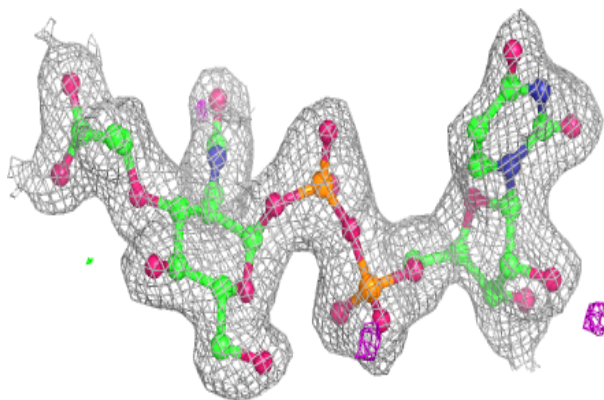
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 87E C 301:**

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

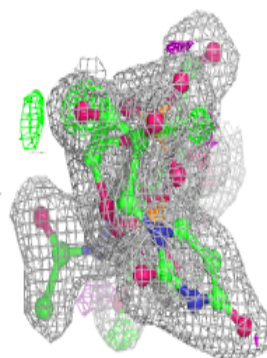
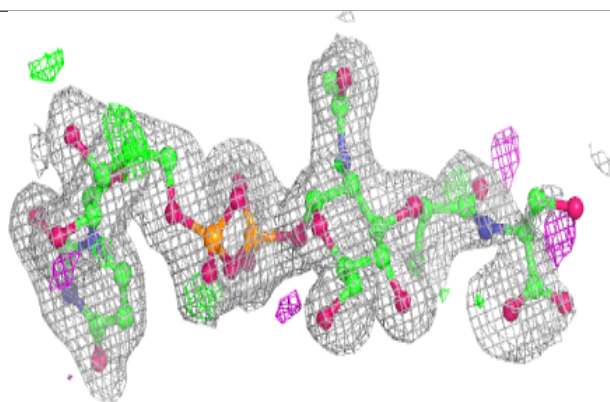
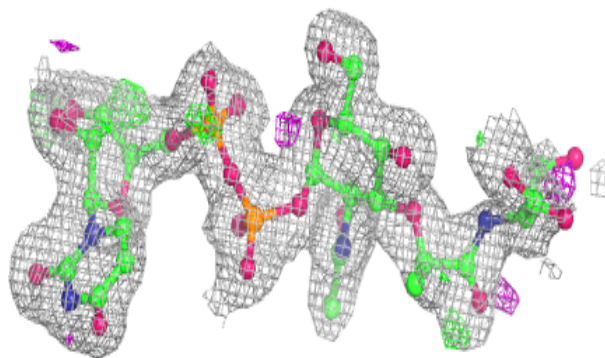
**Electron density around EPZ A 301:**

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

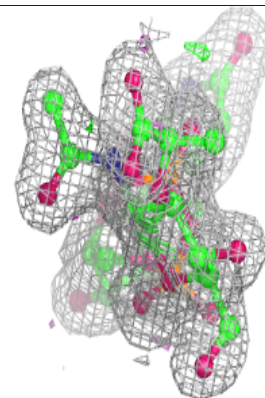
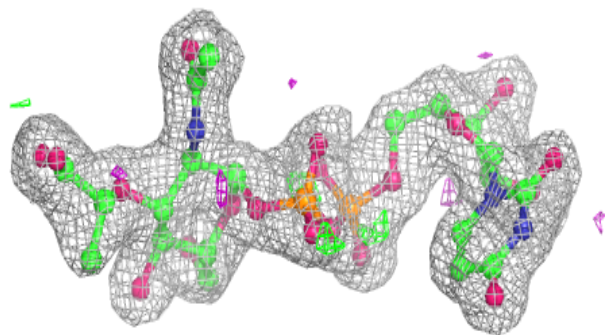
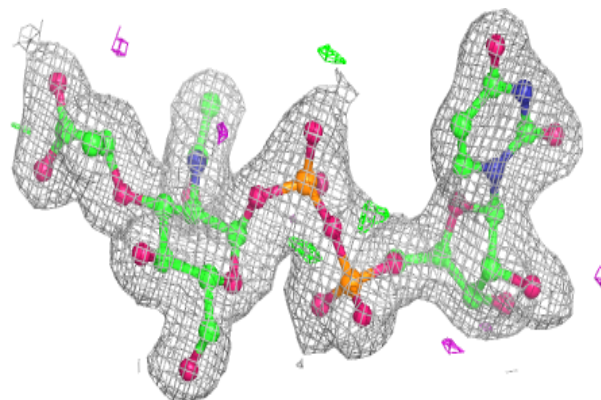


**Electron density around 87E D 301:**

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

**Electron density around EPZ B 301:**

$2mF_o-DF_c$  (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.