



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:02 AM UTC

PDB ID : 9U4I / pdb_00009u4i
Title : Serine Beta-Lactamase OXA-48 in complex with Dual MBL/SBL inhibitor FB1-1
Authors : Li, G.-B.; Liang, G.-Q.
Deposited on : 2025-03-19
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

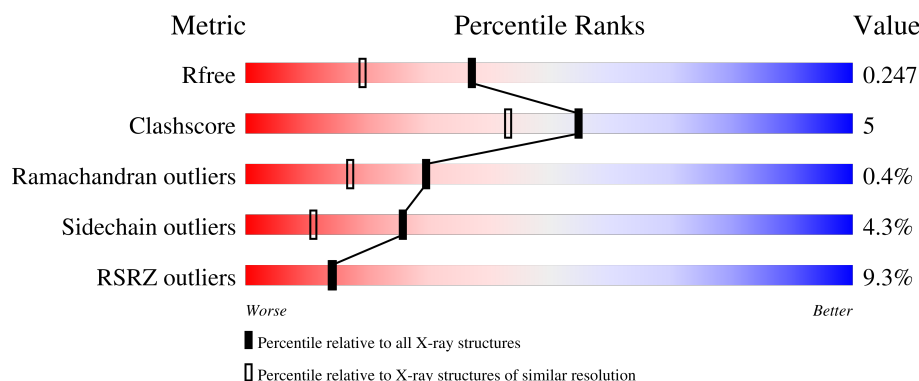
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 ≥ 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	242	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 89% 10% </div> </div>
1	B	242	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 12% </div> </div>
1	C	242	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 26% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 81% 17% </div> </div>
1	D	242	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 7% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 87% 12% </div> </div>

2 Entry composition [i](#)

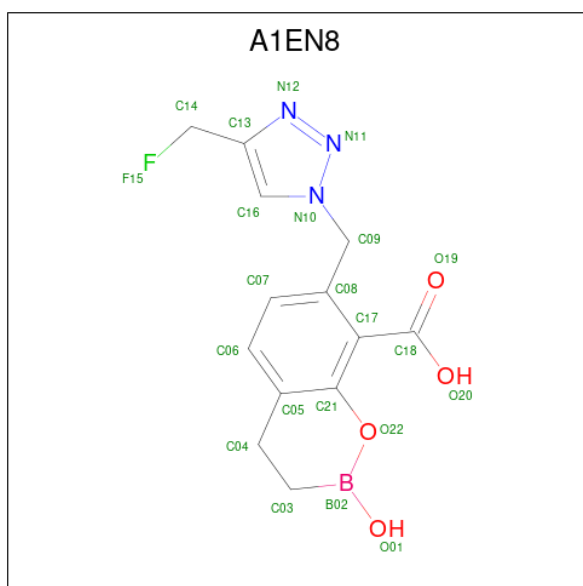
There are 3 unique types of molecules in this entry. The entry contains 16327 atoms, of which 7779 are hydrogens and 0 are deuteriums.

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 Beta-lactamase OXA-48.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	242	Total	C	H	N	O	S		0	0	0
			3916	1262	1933	349	365	7				
1	B	242	Total	C	H	N	O	S		0	0	0
			3915	1262	1932	349	365	7				
1	C	242	Total	C	H	N	O	S		0	0	0
			3916	1262	1933	349	365	7				
1	D	242	Total	C	H	N	O	S		0	0	0
			3916	1262	1933	349	365	7				

- Molecule 2 is 7-[[4-(fluoranylmethyl)-1,2,3-triazol-1-yl]methyl]-2-oxidanyl-3,4-dihydro-1,2-benzoxaborinine-8-carboxylic acid (CCD ID: A1EN8) (formula: C₁₃H₁₃BFN₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	B	C	F	H	N	O	0	0
			34	1	13	1	12	3	4		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	B	1	Total	B	C	F	H	N	O	0	0
			34	1	13	1	12	3	4		
2	C	1	Total	B	C	F	H	N	O	0	0
			34	1	13	1	12	3	4		
2	D	1	Total	B	C	F	H	N	O	0	0
			34	1	13	1	12	3	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		
3	B	168	Total	O	0	0
			168	168		
3	C	85	Total	O	0	0
			85	85		
3	D	114	Total	O	0	0
			114	114		

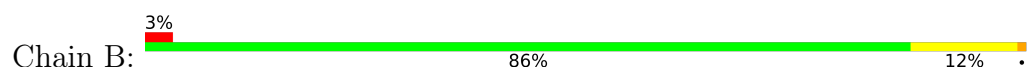
3 Residue-property plots [i](#)

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.

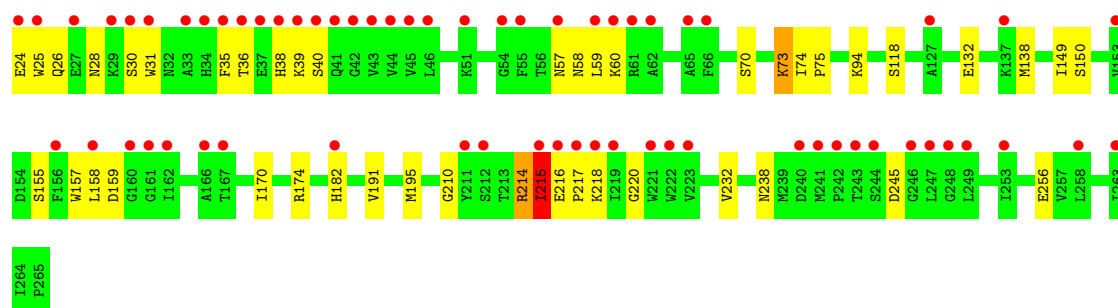
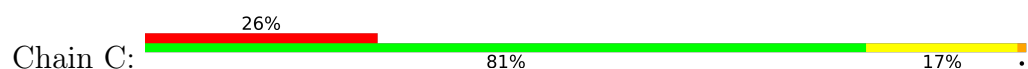
• Molecule 1: Beta-lactamase OXA-48



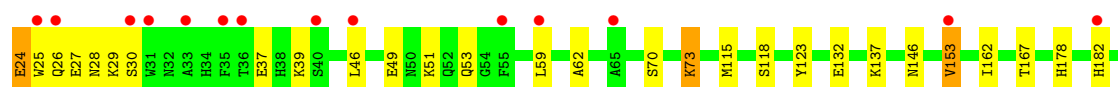
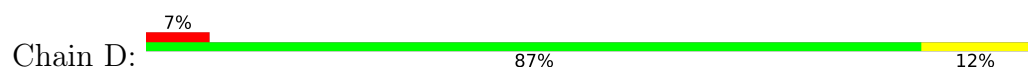
• Molecule 1: Beta-lactamase OXA-48

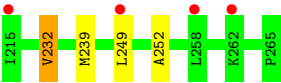


• Molecule 1: Beta-lactamase OXA-48



• Molecule 1: Beta-lactamase OXA-48





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.81Å 56.26Å 102.58Å 90.00° 105.27° 90.00°	Depositor
Resolution (Å)	49.77 – 1.85 49.77 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.77-1.85) 99.2 (49.77-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.201 , 0.242 0.208 , 0.247	Depositor DCC
R_{free} test set	2010 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16327	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: A1EN8, KCX

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	0.66	0/2019	0.72	0/2730
1	B	0.64	0/2019	0.73	1/2730 (0.0%)
1	C	0.49	0/2019	0.62	0/2730
1	D	0.52	0/2019	0.65	0/2730
All	All	0.58	0/8076	0.68	1/10920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	TRP	CA-CB-CG	5.07	123.24	113.60

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	1983	1933	1931	17	0
1	B	1983	1932	1931	19	0
1	C	1983	1933	1931	19	0
1	D	1983	1933	1932	22	0
2	A	22	12	0	4	0
2	B	22	12	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	22	12	0	2	0
2	D	22	12	0	3	0
3	A	161	0	0	1	1
3	B	168	0	0	0	0
3	C	85	0	0	0	1
3	D	114	0	0	2	0
All	All	8548	7779	7725	76	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:SER:OG	2:C:301:A1EN8:O22	1.84	0.96
1:C:70:SER:OG	2:C:301:A1EN8:O01	1.93	0.85
1:C:28:ASN:OD1	1:C:30:SER:OG	2.08	0.72
1:B:101:ASP:OD1	1:B:101:ASP:N	2.23	0.71
1:D:70:SER:HG	2:D:301:A1EN8:C03	2.07	0.67
1:B:70:SER:OG	2:B:301:A1EN8:O22	2.13	0.65
1:D:70:SER:OG	2:D:301:A1EN8:O22	2.15	0.63
1:D:28:ASN:OD1	1:D:30:SER:OG	2.16	0.63
1:A:70:SER:OG	2:A:301:A1EN8:O22	2.20	0.59
1:A:33:ALA:O	1:A:37:GLU:HG2	2.02	0.58
1:D:132:GLU:OE1	1:D:153:VAL:HG22	2.02	0.58
1:C:216:GLU:OE2	1:C:217:PRO:HA	2.04	0.58
1:A:70:SER:OG	2:A:301:A1EN8:C03	2.51	0.58
1:C:216:GLU:OE1	1:C:218:LYS:NZ	2.32	0.57
1:B:70:SER:OG	2:B:301:A1EN8:C03	2.53	0.56
1:A:250:ARG:HH12	2:A:301:A1EN8:C16	2.19	0.56
1:C:70:SER:HA	1:C:73:KCX:CX	2.35	0.56
1:D:182:HIS:O	1:D:182:HIS:CG	2.58	0.55
1:D:178:HIS:ND1	3:D:401:HOH:O	2.33	0.55
1:D:70:SER:OG	2:D:301:A1EN8:C03	2.55	0.55
1:A:216:GLU:OE1	1:A:218:LYS:NZ	2.37	0.54
1:A:31:TRP:HB2	1:A:57:ASN:HB3	1.89	0.54
1:D:24:GLU:HA	1:D:24:GLU:OE1	2.09	0.53
1:A:70:SER:OG	2:A:301:A1EN8:O01	2.27	0.53
1:C:170:ILE:O	1:C:174:ARG:HG3	2.08	0.53
1:D:115:MET:HG2	1:D:123:TYR:OH	2.10	0.52
1:C:24:GLU:O	1:C:26:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ILE:O	1:C:150:SER:C	2.55	0.50
1:D:239:MET:HE1	1:D:249:LEU:HB2	1.92	0.50
1:C:157:TRP:CD1	1:C:158:LEU:HG	2.48	0.49
1:B:70:SER:OG	2:B:301:A1EN8:O01	2.31	0.49
1:D:25:TRP:O	1:D:26:GLN:HG3	2.13	0.49
1:B:220:GLY:O	1:B:238:ASN:HA	2.13	0.48
1:D:249:LEU:HA	1:D:252:ALA:HB3	1.94	0.48
1:C:138:MET:SD	1:C:182:HIS:CE1	3.06	0.48
1:D:137:LYS:HG3	3:D:437:HOH:O	2.14	0.48
1:A:220:GLY:O	1:A:238:ASN:HA	2.12	0.48
1:C:220:GLY:O	1:C:238:ASN:HA	2.12	0.48
1:A:24:GLU:N	1:B:24:GLU:HB3	2.29	0.47
1:D:182:HIS:O	1:D:182:HIS:ND1	2.47	0.47
1:D:132:GLU:CD	1:D:153:VAL:HG22	2.40	0.47
1:B:70:SER:CB	2:B:301:A1EN8:O22	2.63	0.46
1:A:140:HIS:CD2	1:A:147:GLU:OE1	2.68	0.46
1:B:48:ASN:HB2	1:B:233:TRP:CH2	2.51	0.46
1:C:70:SER:HB2	1:C:210:GLY:HA2	1.98	0.46
1:C:74:ILE:HB	1:C:75:PRO:CD	2.46	0.46
1:C:36:THR:C	1:C:38:HIS:H	2.24	0.45
1:D:27:GLU:OE2	1:D:29:LYS:HE3	2.17	0.45
1:C:35:PHE:HB3	1:C:40:SER:O	2.17	0.45
1:A:48:ASN:HB2	1:A:233:TRP:CH2	2.52	0.45
1:A:24:GLU:CB	3:A:422:HOH:O	2.65	0.44
1:B:36:THR:C	1:B:38:HIS:N	2.74	0.44
1:A:170:ILE:O	1:A:174:ARG:HG3	2.16	0.44
1:A:31:TRP:CH2	1:A:46:LEU:HD22	2.53	0.44
1:B:73:KCX:OQ1	1:B:157:TRP:NE1	2.50	0.44
1:B:65:ALA:HB1	1:B:163:ARG:HB3	1.99	0.43
1:B:73:KCX:HE2	1:B:118:SER:C	2.44	0.43
1:B:132:GLU:CG	1:B:153:VAL:HG22	2.48	0.43
1:A:45:VAL:O	1:A:235:PHE:HA	2.18	0.43
1:B:24:GLU:HG3	1:B:52:GLN:O	2.19	0.43
1:B:80:ALA:HB1	1:B:86:VAL:HG23	1.99	0.43
1:B:31:TRP:HB2	1:B:57:ASN:HB3	2.00	0.42
1:D:49:GLU:CB	1:D:232:VAL:HG13	2.50	0.42
1:A:95:TRP:HB2	1:A:107:ARG:C	2.44	0.42
1:D:146:ASN:C	1:D:146:ASN:OD1	2.62	0.42
1:D:62:ALA:O	1:D:167:THR:HG23	2.20	0.41
1:D:115:MET:HE3	1:D:115:MET:HB3	1.86	0.41
1:D:73:KCX:HE2	1:D:123:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:N	1:B:121:PRO:HD2	2.36	0.41
1:C:214:ARG:O	1:C:215:ILE:CG1	2.69	0.41
1:C:191:VAL:O	1:C:195:MET:HG3	2.20	0.41
1:A:27:GLU:HA	1:A:56:THR:O	2.20	0.41
1:C:31:TRP:HB2	1:C:57:ASN:HB3	2.03	0.41
1:B:70:SER:CB	2:B:301:A1EN8:O01	2.68	0.41
1:B:115:MET:HE3	1:B:115:MET:HB3	1.94	0.40
1:D:51:LYS:O	1:D:53:GLN:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:419:HOH:O	3:C:440:HOH:O[1_545]	2.05	0.15

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	239/242 (99%)	234 (98%)	5 (2%)	0	100	100
1	B	239/242 (99%)	232 (97%)	7 (3%)	0	100	100
1	C	239/242 (99%)	222 (93%)	13 (5%)	4 (2%)	7	1
1	D	239/242 (99%)	230 (96%)	9 (4%)	0	100	100
All	All	956/968 (99%)	918 (96%)	34 (4%)	4 (0%)	30	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	TRP
1	C	159	ASP

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Mol	Chain	Res	Type
1	C	58	ASN
1	C	215	ILE

5.3.2 Protein sidechains ⓘ

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	210/210 (100%)	205 (98%)	5 (2%)	43	28
1	B	210/210 (100%)	200 (95%)	10 (5%)	23	8
1	C	210/210 (100%)	198 (94%)	12 (6%)	18	6
1	D	210/210 (100%)	201 (96%)	9 (4%)	26	11
All	All	840/840 (100%)	804 (96%)	36 (4%)	26	11

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	37	GLU
1	A	46	LEU
1	A	125	GLU
1	A	153	VAL
1	B	46	LEU
1	B	60	LYS
1	B	94	LYS
1	B	101	ASP
1	B	118	SER
1	B	125	GLU
1	B	137	LYS
1	B	180	LYS
1	B	230	ASP
1	B	232	VAL
1	C	39	LYS
1	C	59	LEU
1	C	60	LYS
1	C	94	LYS

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Mol	Chain	Res	Type
1	C	118	SER
1	C	132	GLU
1	C	155	SER
1	C	214	ARG
1	C	215	ILE
1	C	232	VAL
1	C	245	ASP
1	C	256	GLU
1	D	24	GLU
1	D	37	GLU
1	D	39	LYS
1	D	46	LEU
1	D	59	LEU
1	D	118	SER
1	D	153	VAL
1	D	162	ILE
1	D	232	VAL

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

Mol	Chain	Res	Type
1	A	90	HIS
1	B	26	GLN
1	B	90	HIS
1	C	52	GLN
1	D	52	GLN
1	D	64	GLN
1	D	90	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	KCX	D	73	1	10,11,12	1.40	2 (20%)	6,12,14	0.75	0
1	KCX	B	73	1	10,11,12	2.08	4 (40%)	6,12,14	3.43	2 (33%)
1	KCX	A	73	1	10,11,12	1.90	4 (40%)	6,12,14	0.64	0
1	KCX	C	73	1	10,11,12	1.19	2 (20%)	6,12,14	3.59	2 (33%)

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
1	KCX	D	73	1	-	0/9/10/12	-
1	KCX	B	73	1	-	1/9/10/12	-
1	KCX	A	73	1	-	0/9/10/12	-
1	KCX	C	73	1	-	2/9/10/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	KCX	CX-NZ	-4.02	1.28	1.35
1	B	73	KCX	CX-NZ	-3.90	1.28	1.35
1	B	73	KCX	CE-NZ	-3.55	1.38	1.46
1	B	73	KCX	OQ1-CX	-3.02	1.16	1.21
1	D	73	KCX	OQ1-CX	-2.55	1.17	1.21
1	A	73	KCX	CA-N	-2.54	1.40	1.48
1	A	73	KCX	CB-CA	-2.42	1.49	1.53
1	C	73	KCX	OQ1-CX	-2.31	1.17	1.21
1	C	73	KCX	CA-N	-2.30	1.41	1.48
1	B	73	KCX	CA-N	-2.07	1.42	1.48
1	A	73	KCX	OQ1-CX	-2.05	1.18	1.21
1	D	73	KCX	CA-N	-2.03	1.42	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	KCX	OQ1-CX-NZ	-8.08	112.65	124.92
1	B	73	KCX	OQ1-CX-NZ	-7.29	113.84	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	KCX	CE-NZ-CX	3.58	128.05	121.98
1	C	73	KCX	CD-CE-NZ	2.93	120.43	112.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	73	KCX	OQ1-CX-NZ-CE
1	C	73	KCX	CG-CD-CE-NZ
1	C	73	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	73	KCX	1	0
1	B	73	KCX	2	0
1	C	73	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	A1EN8	B	301	-	20,24,24	1.47	3 (15%)	25,34,34	1.67	6 (24%)
2	A1EN8	C	301	-	20,24,24	1.60	3 (15%)	25,34,34	1.94	6 (24%)
2	A1EN8	D	301	-	20,24,24	1.66	4 (20%)	25,34,34	1.62	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1EN8	A	301	-	20,24,24	1.49	2 (10%)	25,34,34	2.87	9 (36%)

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	A1EN8	B	301	-	-	0/8/19/19	0/2/3/3
2	A1EN8	C	301	-	-	0/8/19/19	0/2/3/3
2	A1EN8	D	301	-	-	1/8/19/19	0/2/3/3
2	A1EN8	A	301	-	-	2/8/19/19	0/2/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1EN8	C16-C13	4.68	1.44	1.36
2	C	301	A1EN8	C16-C13	4.63	1.44	1.36
2	B	301	A1EN8	C16-C13	4.45	1.43	1.36
2	A	301	A1EN8	C16-C13	4.32	1.43	1.36
2	C	301	A1EN8	O22-C21	3.16	1.44	1.38
2	A	301	A1EN8	O22-C21	3.03	1.44	1.38
2	D	301	A1EN8	C04-C05	2.89	1.56	1.51
2	D	301	A1EN8	O22-C21	2.82	1.43	1.38
2	B	301	A1EN8	O22-C21	2.62	1.43	1.38
2	D	301	A1EN8	C09-C08	2.59	1.56	1.51
2	C	301	A1EN8	C04-C05	2.48	1.55	1.51
2	B	301	A1EN8	C09-N10	-2.02	1.43	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1EN8	C09-N10-N11	7.97	131.22	120.03
2	A	301	A1EN8	O22-C21-C17	5.33	124.69	119.28
2	C	301	A1EN8	O22-C21-C17	4.82	124.17	119.28
2	A	301	A1EN8	C16-N10-N11	-4.77	106.11	110.75
2	D	301	A1EN8	N10-N11-N12	4.42	111.00	107.02
2	A	301	A1EN8	C09-N10-C16	-4.16	122.66	128.65
2	A	301	A1EN8	C16-C13-N12	-3.98	103.28	108.12
2	B	301	A1EN8	N10-N11-N12	3.87	110.50	107.02
2	A	301	A1EN8	C13-C16-N10	3.80	110.65	105.33
2	C	301	A1EN8	C09-N10-N11	3.77	125.33	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1EN8	N10-N11-N12	3.77	110.41	107.02
2	B	301	A1EN8	C09-N10-N11	3.76	125.31	120.03
2	C	301	A1EN8	N10-N11-N12	3.65	110.31	107.02
2	C	301	A1EN8	O20-C18-O19	-2.72	117.50	123.35
2	D	301	A1EN8	C16-N10-N11	-2.72	108.11	110.75
2	B	301	A1EN8	C06-C05-C21	2.63	121.74	117.88
2	B	301	A1EN8	C07-C06-C05	-2.60	117.99	121.39
2	A	301	A1EN8	C06-C05-C21	2.57	121.65	117.88
2	D	301	A1EN8	C09-N10-N11	2.56	123.62	120.03
2	C	301	A1EN8	C09-N10-C16	-2.54	125.00	128.65
2	D	301	A1EN8	O22-C21-C17	2.51	121.83	119.28
2	D	301	A1EN8	O20-C18-O19	-2.33	118.35	123.35
2	B	301	A1EN8	O22-C21-C17	2.26	121.58	119.28
2	C	301	A1EN8	C06-C05-C21	2.21	121.12	117.88
2	A	301	A1EN8	C17-C21-C05	-2.16	118.23	121.87
2	B	301	A1EN8	C09-N10-C16	-2.06	125.69	128.65
2	D	301	A1EN8	C07-C06-C05	-2.03	118.73	121.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1EN8	C08-C09-N10-N11
2	A	301	A1EN8	C08-C09-N10-C16
2	D	301	A1EN8	C08-C09-N10-N11

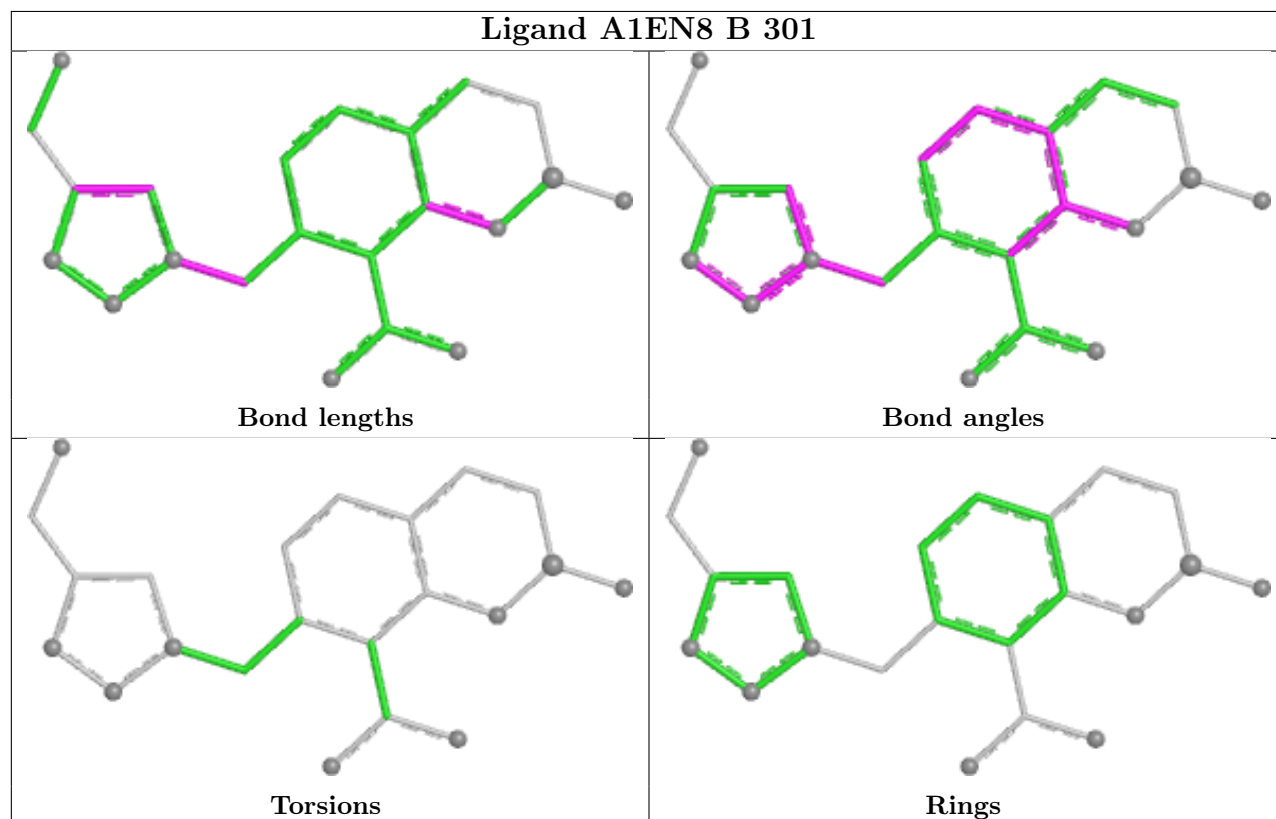
There are no ring outliers.

4 monomers are involved in 14 short contacts:

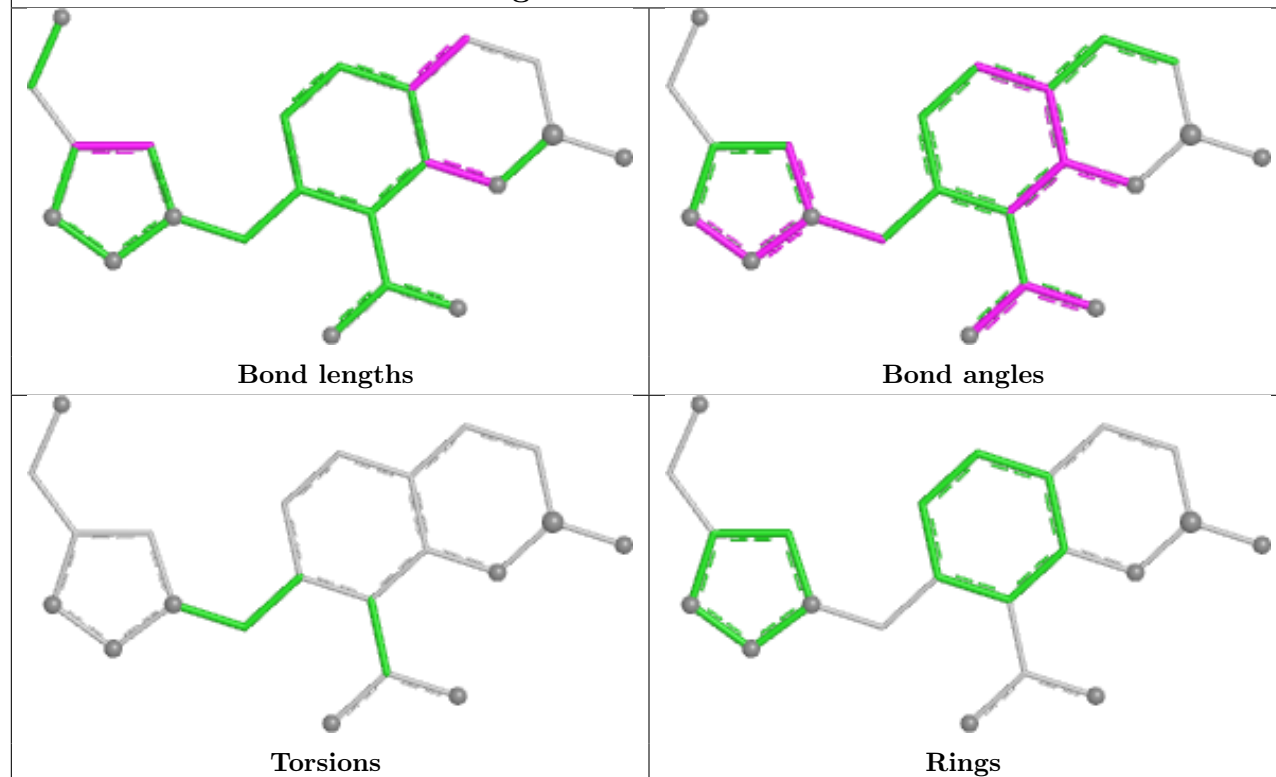
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	A1EN8	5	0
2	C	301	A1EN8	2	0
2	D	301	A1EN8	3	0
2	A	301	A1EN8	4	0

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

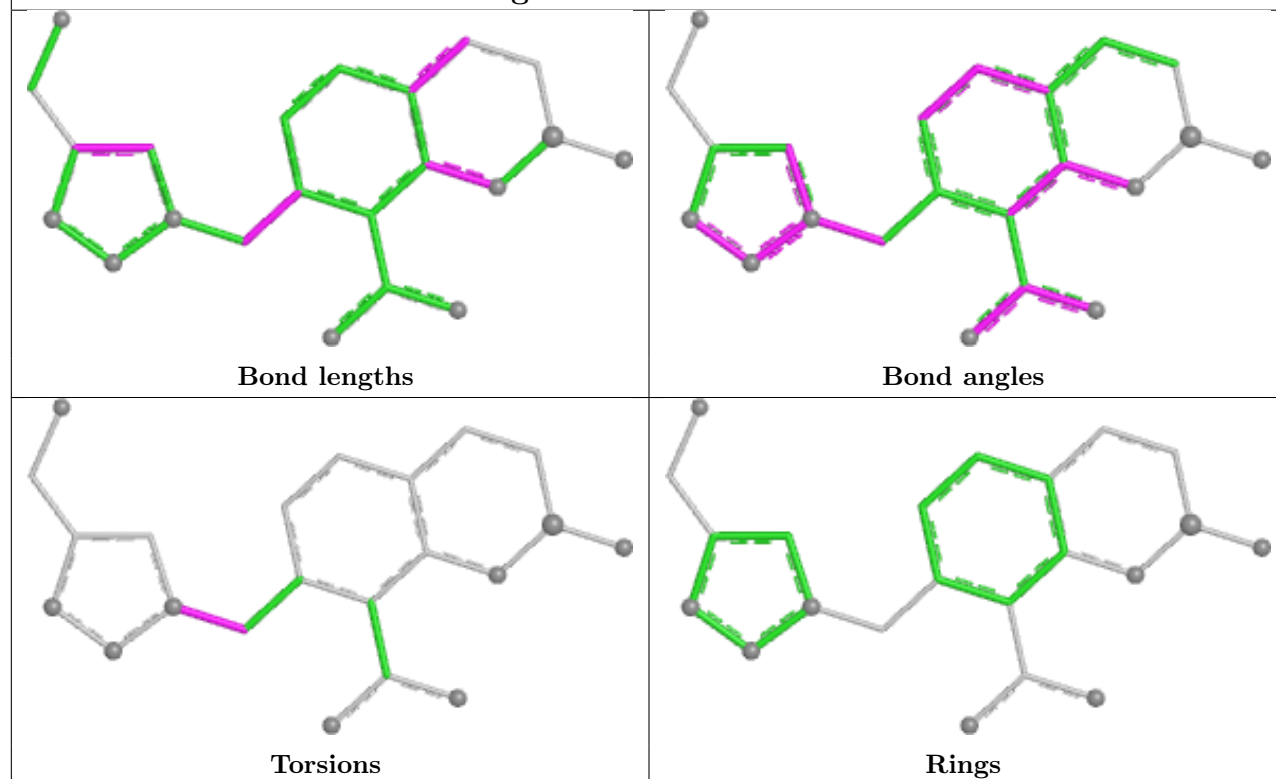
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

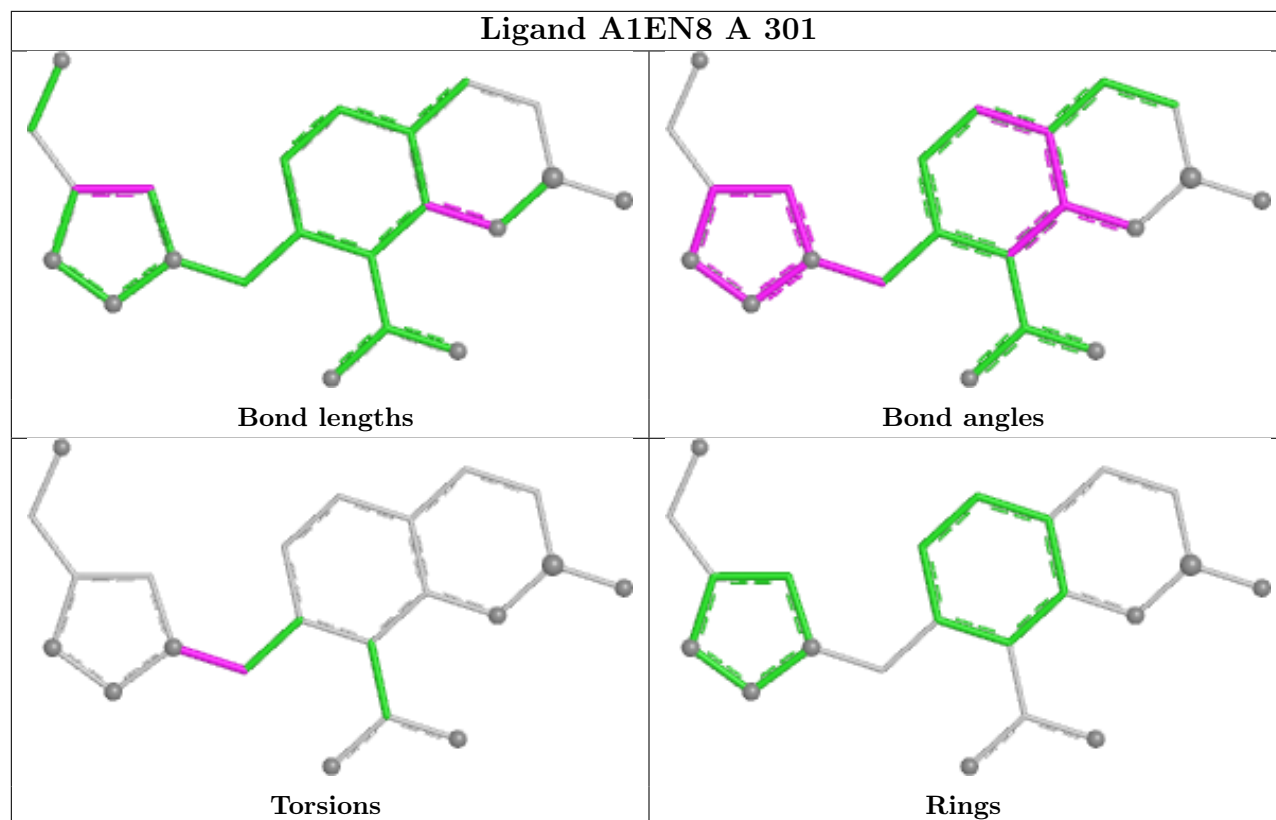


Ligand A1EN8 C 301



Ligand A1EN8 D 301





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	241/242 (99%)	-0.07	2 (0%) 82 86	20, 31, 44, 58	0
1	B	241/242 (99%)	0.07	7 (2%) 53 57	23, 32, 49, 67	0
1	C	241/242 (99%)	1.30	63 (26%) 1 1	27, 51, 78, 92	0
1	D	241/242 (99%)	0.58	18 (7%) 20 22	23, 42, 68, 80	0
All	All	964/968 (99%)	0.47	90 (9%) 14 14	20, 37, 68, 92	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	PRO	5.7
1	C	215	ILE	5.6
1	C	219	ILE	4.8
1	C	25	TRP	4.5
1	B	36	THR	4.5
1	D	25	TRP	3.9
1	C	161	GLY	3.9
1	B	33	ALA	3.7
1	C	41	GLN	3.6
1	C	65	ALA	3.6
1	C	162	ILE	3.6
1	C	182	HIS	3.5
1	C	167	THR	3.5
1	C	35	PHE	3.5
1	C	38	HIS	3.5
1	D	33	ALA	3.5
1	C	153	VAL	3.4
1	C	40	SER	3.4
1	C	59	LEU	3.4
1	B	182	HIS	3.3
1	C	62	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	166	ALA	3.3
1	C	211	TYR	3.2
1	C	43	VAL	3.1
1	C	247	LEU	3.1
1	C	218	LYS	3.1
1	C	243	THR	3.1
1	C	31	TRP	3.1
1	D	59	LEU	3.1
1	C	29	LYS	3.0
1	C	249	LEU	3.0
1	C	137	LYS	3.0
1	D	35	PHE	3.0
1	C	55	PHE	2.9
1	B	153	VAL	2.9
1	C	33	ALA	2.9
1	C	60	LYS	2.8
1	C	46	LEU	2.8
1	C	244	SER	2.7
1	C	39	LYS	2.7
1	C	54	GLY	2.7
1	D	182	HIS	2.7
1	C	242	PRO	2.7
1	C	222	TRP	2.6
1	D	55	PHE	2.6
1	C	156	PHE	2.6
1	C	212	SER	2.6
1	A	24	GLU	2.5
1	C	66	PHE	2.5
1	C	158	LEU	2.5
1	C	246	GLY	2.4
1	A	182	HIS	2.4
1	C	253	ILE	2.4
1	D	26	GLN	2.4
1	D	30	SER	2.4
1	C	45	VAL	2.4
1	C	34	HIS	2.4
1	C	241	MET	2.4
1	B	39	LYS	2.4
1	D	65	ALA	2.4
1	C	42	GLY	2.4
1	D	249	LEU	2.3
1	C	248	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	262	LYS	2.3
1	C	30	SER	2.3
1	C	240	ASP	2.2
1	C	223	VAL	2.2
1	C	263	ILE	2.2
1	D	31	TRP	2.2
1	B	24	GLU	2.2
1	C	36	THR	2.2
1	B	101	ASP	2.2
1	C	57	ASN	2.1
1	C	160	GLY	2.1
1	D	215	ILE	2.1
1	C	221	TRP	2.1
1	C	37	GLU	2.1
1	C	216	GLU	2.1
1	D	40	SER	2.1
1	C	51	LYS	2.1
1	C	44	VAL	2.1
1	C	258	LEU	2.1
1	C	61	ARG	2.1
1	C	24	GLU	2.0
1	C	27	GLU	2.0
1	D	36	THR	2.0
1	D	153	VAL	2.0
1	D	46	LEU	2.0
1	D	258	LEU	2.0
1	C	127	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	C	73	12/13	0.85	0.12	27,41,54,65	0
1	KCX	B	73	12/13	0.91	0.10	19,27,44,49	0
1	KCX	A	73	12/13	0.96	0.06	21,27,31,34	0
1	KCX	D	73	12/13	0.96	0.06	23,30,35,37	0

6.3 Carbohydrates [i](#)

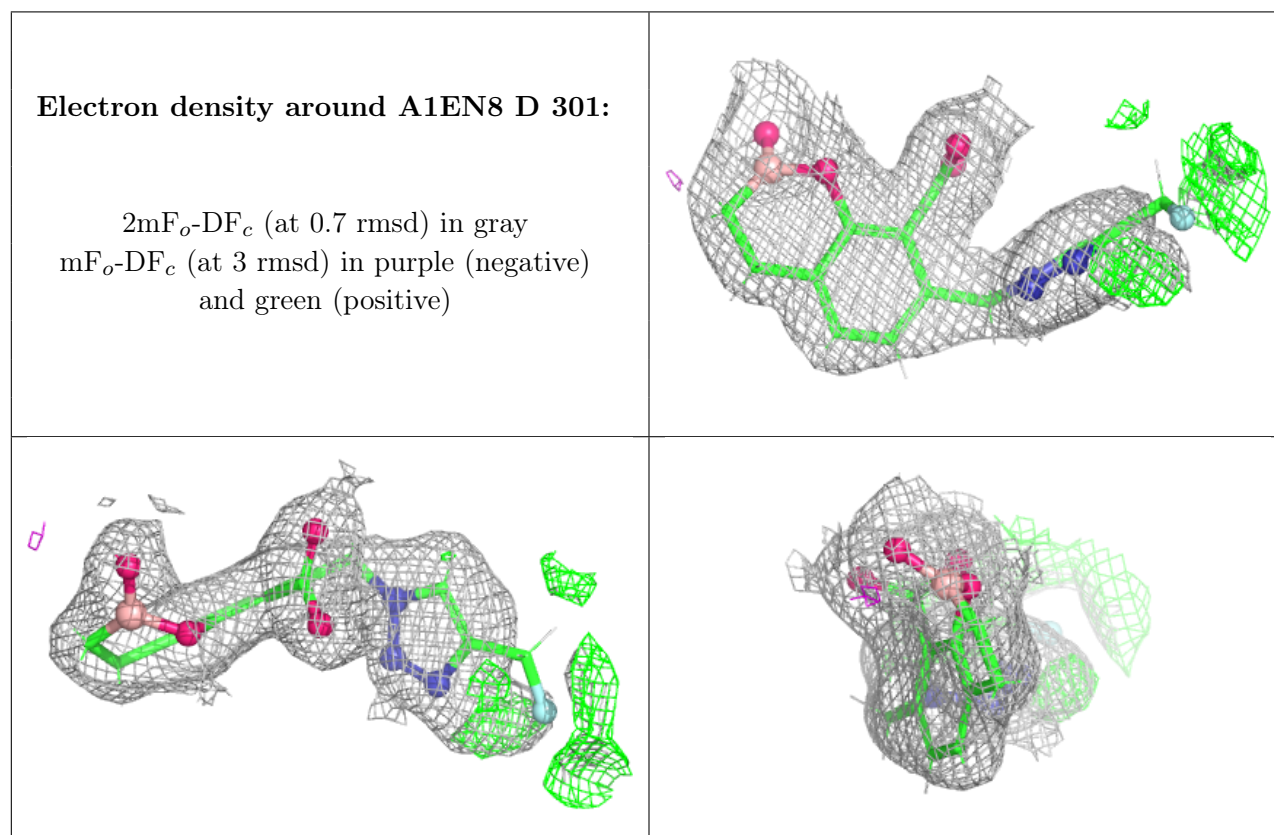
There are no oligosaccharides in this entry.

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, 95th 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.

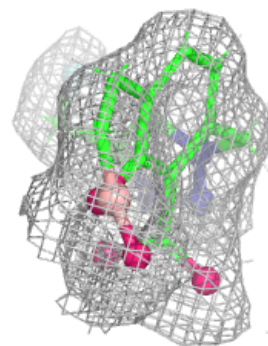
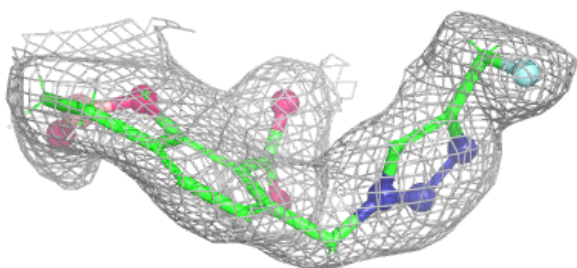
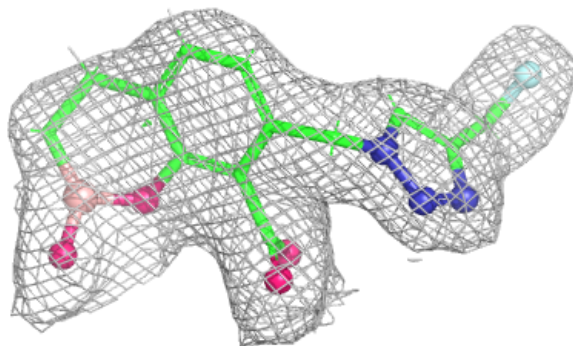
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1EN8	D	301	22/22	0.90	0.11	29,38,74,76	0
2	A1EN8	C	301	22/22	0.92	0.10	37,48,57,58	0
2	A1EN8	A	301	22/22	0.94	0.08	22,30,49,58	0
2	A1EN8	B	301	22/22	0.95	0.08	22,30,45,48	0

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.

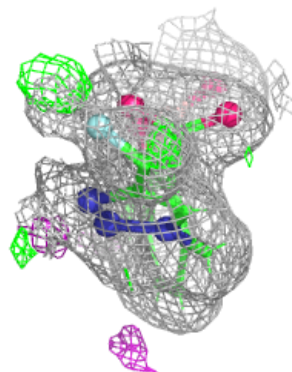
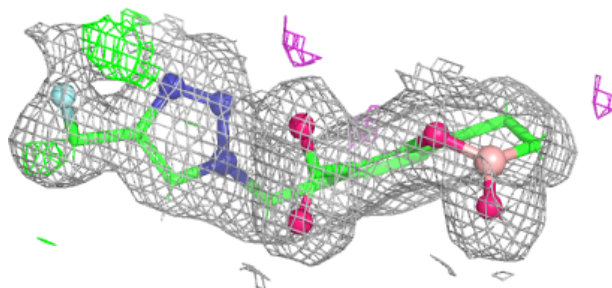
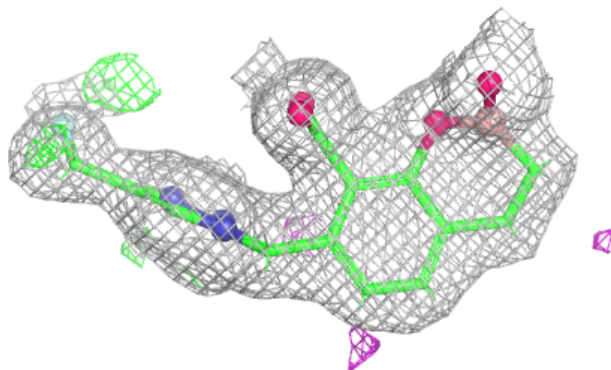


Electron density around A1EN8 C 301:

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

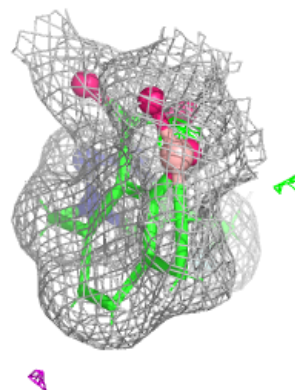
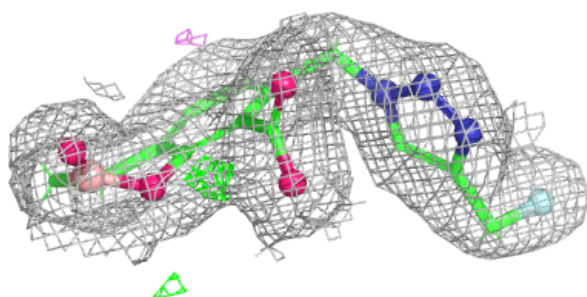
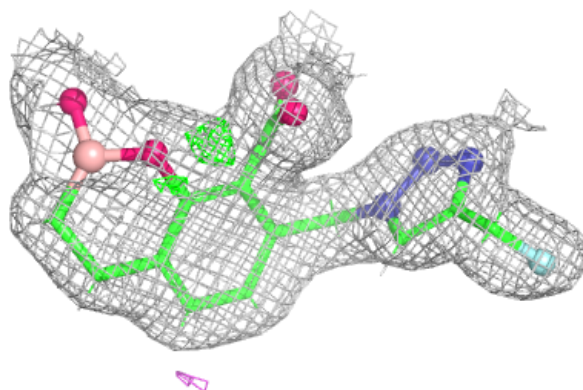
**Electron density around A1EN8 A 301:**

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



Electron density around A1EN8 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 ⓘ

There are no such residues in this entry.