Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2025 – 01:28 pm BST

PDB ID	:	9FNV / pdb_00009fnv
Title	:	Structure of the mouse 8-oxoguanine DNA Glycosylase mOGG1 in complex with ligand TH12163
Authors	:	Scaletti, E.; Davies, J.R.; Stenmark, P.
Deposited on	:	2024-06-11
Resolution	:	2.25 Å(reported)

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

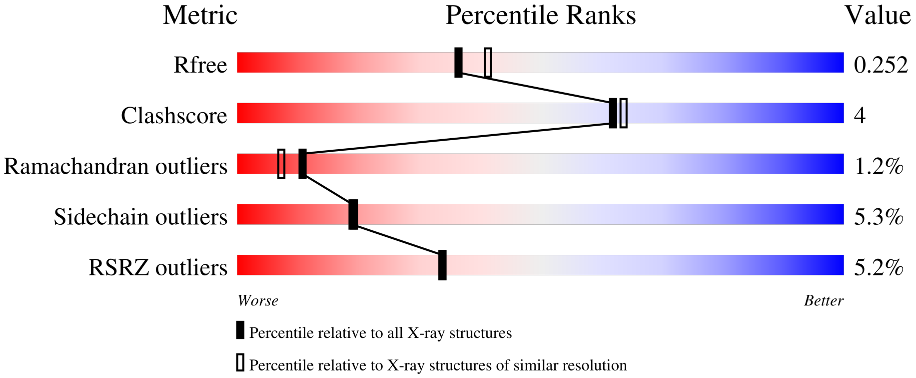
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

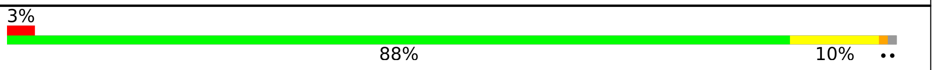
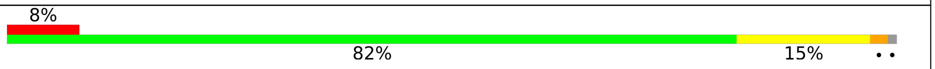
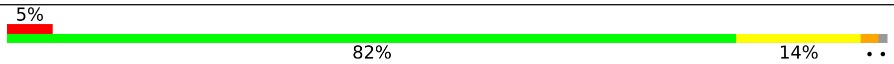
The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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 <=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	318	
1	B	318	
1	C	318	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15228 atoms, of which 7448 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.

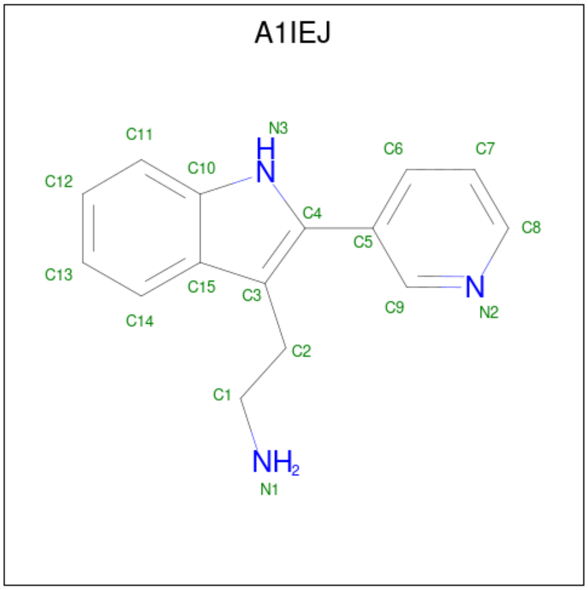
- Molecule 1 is a protein called N-glycosylase/DNA lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	H	N	O	S	79	0	0
			4972	1594	2466	453	448	11			
1	B	316	Total	C	H	N	O	S	79	0	0
			4989	1599	2474	455	450	11			
1	C	315	Total	C	H	N	O	S	79	0	0
			4964	1591	2463	452	447	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP O08760
A	9	SER	-	expression tag	UNP O08760
A	10	HIS	-	expression tag	UNP O08760
B	8	GLY	-	expression tag	UNP O08760
B	9	SER	-	expression tag	UNP O08760
B	10	HIS	-	expression tag	UNP O08760
C	8	GLY	-	expression tag	UNP O08760
C	9	SER	-	expression tag	UNP O08760
C	10	HIS	-	expression tag	UNP O08760

- Molecule 2 is 2-(2-pyridin-3-yl-1 {H}-indol-3-yl)ethanamine (CCD ID: A1IEJ) (formula: $C_{15}H_{15}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H N 33 15 15 3	0	0
2	B	1	Total C H N 33 15 15 3	0	0
2	C	1	Total C H N 33 15 15 3	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- Molecule 4 is water.

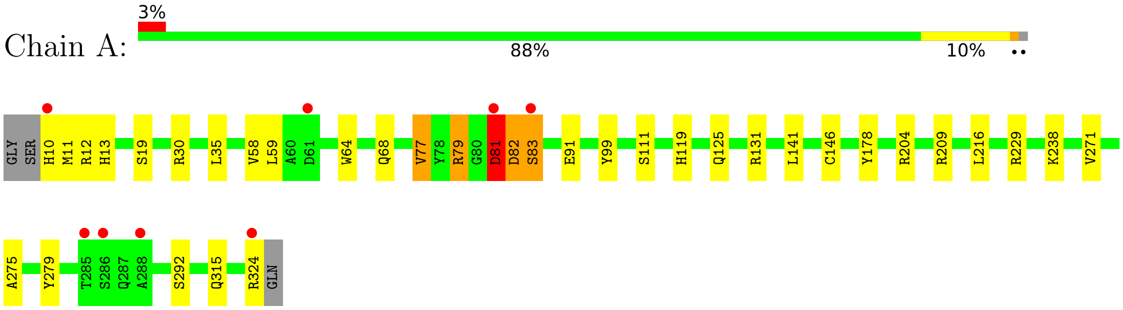
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0
4	B	44	Total O 44 44	0	0
4	C	50	Total O 50 50	0	0

3 Residue-property plots

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.

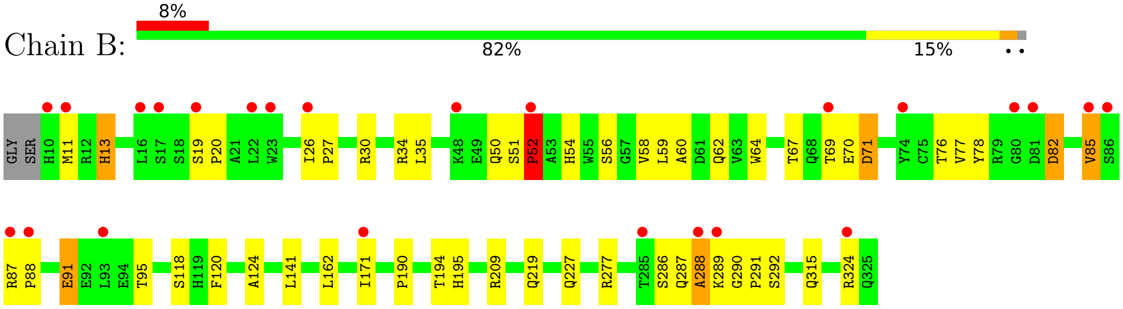
- Molecule 1: N-glycosylase/DNA lyase

Chain A:



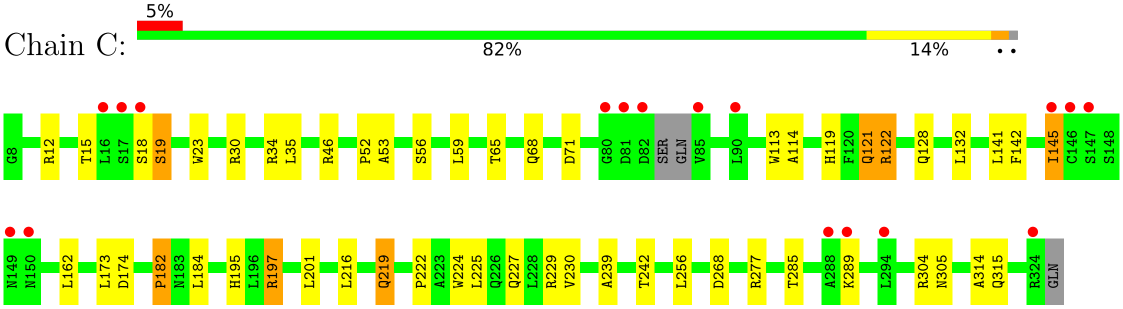
- Molecule 1: N-glycosylase/DNA lyase

Chain B:



- Molecule 1: N-glycosylase/DNA lyase

Chain C:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.39Å 81.48Å 170.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.40 – 2.25 73.40 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.40-2.25) 100.0 (73.40-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.200 , 0.252 0.200 , 0.252	Depositor DCC
R_{free} test set	2582 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15228	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NI, A1IEJ

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	0.68	0/2577	1.08	1/3508 (0.0%)
1	B	0.61	0/2586	1.07	2/3520 (0.1%)
1	C	0.61	0/2571	1.08	3/3498 (0.1%)
All	All	0.63	0/7734	1.08	6/10526 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	4
1	C	0	5
All	All	0	17

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	195	HIS	CA-CB-CG	6.85	120.65	113.80
1	A	292	SER	N-CA-C	-5.98	102.75	108.13
1	C	268	ASP	CA-CB-CG	5.89	118.50	112.60
1	B	52	PRO	N-CA-CB	-5.45	97.53	103.25
1	B	195	HIS	CA-CB-CG	5.37	119.17	113.80
1	C	182	PRO	CB-CA-C	-5.33	104.57	111.39

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	209	ARG	Sidechain
1	A	229	ARG	Sidechain
1	A	30	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	81	ASP	Peptide
1	A	82	ASP	Peptide
1	B	209	ARG	Sidechain
1	B	277	ARG	Sidechain
1	B	70	GLU	Peptide
1	B	87	ARG	Sidechain
1	C	122	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	229	ARG	Sidechain
1	C	277	ARG	Sidechain
1	C	304	ARG	Sidechain

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	2506	2466	2452	13	0
1	B	2515	2474	2460	19	0
1	C	2501	2463	2446	28	0
2	A	18	15	0	0	0
2	B	18	15	0	0	0
2	C	18	15	0	0	0
3	A	1	0	0	0	0
4	A	109	0	0	1	0
4	B	44	0	0	1	0
4	C	50	0	0	7	0
All	All	7780	7448	7358	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:C:285:THR:HA	4:C:531:HOH:O	1.76	0.85
1:C:315:GLN:NE2	4:C:501:HOH:O	2.12	0.82
1:C:56:SER:HG	1:C:65:THR:HG1	1.33	0.74
1:A:81:ASP:O	1:A:83:SER:N	2.22	0.72
1:B:91:GLU:H	1:B:91:GLU:CD	2.02	0.67
1:C:18:SER:O	1:C:19:SER:HB3	1.94	0.66
1:C:113:TRP:CE2	1:C:314:ALA:HB2	2.31	0.65
1:A:13:HIS:HE1	1:A:178:TYR:OH	1.81	0.64
1:C:119:HIS:HE1	4:C:535:HOH:O	1.81	0.62
1:C:184:LEU:HD12	1:C:222:PRO:HD3	1.84	0.59
1:C:132:LEU:CD2	1:C:256:LEU:HG	2.33	0.58
1:C:114:ALA:HB1	1:C:121:GLN:HG2	1.86	0.56
1:B:162:LEU:C	1:B:162:LEU:HD23	2.30	0.56
1:A:141:LEU:C	1:A:141:LEU:HD23	2.32	0.55
1:A:324:ARG:HH11	1:A:324:ARG:HG3	1.70	0.54
1:C:18:SER:O	1:C:19:SER:CB	2.55	0.54
1:B:288:ALA:C	1:B:290:GLY:H	2.16	0.54
1:C:128:GLN:NE2	4:C:502:HOH:O	2.41	0.53
1:C:35:LEU:H	1:C:68:GLN:HE22	1.59	0.51
1:C:219:GLN:HG2	1:C:224:TRP:CD1	2.46	0.50
1:B:85:VAL:HG12	1:B:85:VAL:O	2.12	0.50
1:B:76:THR:HA	1:B:88:PRO:HG3	1.94	0.49
1:B:52:PRO:O	1:B:54:HIS:CD2	2.64	0.49
1:C:12:ARG:HH11	1:C:12:ARG:HG2	1.78	0.49
1:C:46:ARG:HD2	4:C:504:HOH:O	2.13	0.48
1:A:59:LEU:HD11	1:A:99:TYR:CE1	2.50	0.47
1:A:119:HIS:HE1	4:A:505:HOH:O	1.96	0.47
1:A:324:ARG:HG3	1:A:324:ARG:NH1	2.30	0.47
1:B:26:ILE:HG23	1:B:27:PRO:HD2	1.96	0.47
1:A:35:LEU:H	1:A:68:GLN:HE22	1.63	0.46
1:A:146:CYS:HA	1:A:204:ARG:HD3	1.98	0.46
1:B:13:HIS:CE1	1:B:50:GLN:HG3	2.50	0.46
1:C:162:LEU:HD21	1:C:182:PRO:HG2	1.99	0.45
1:C:52:PRO:O	1:C:53:ALA:HB3	2.17	0.45
1:C:239:ALA:O	1:C:242:THR:HB	2.16	0.45
1:C:30:ARG:HG2	1:C:34:ARG:HG2	1.98	0.45
1:A:13:HIS:CE1	1:A:178:TYR:OH	2.66	0.44
1:B:58:VAL:HA	1:B:62:GLN:O	2.18	0.44
1:B:82:ASP:N	1:B:82:ASP:OD1	2.50	0.44
1:B:324:ARG:NH1	4:B:504:HOH:O	2.50	0.44
1:C:71:ASP:N	1:C:71:ASP:OD1	2.51	0.43
1:B:51:SER:O	1:B:52:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ALA:O	1:A:279:TYR:HB2	2.18	0.43
1:C:227:GLN:O	1:C:230:VAL:HG22	2.18	0.43
1:C:305:ASN:HB2	4:C:538:HOH:O	2.18	0.43
1:C:173:LEU:O	1:C:174:ASP:C	2.61	0.43
1:B:219:GLN:HE21	1:B:219:GLN:HA	1.84	0.42
1:B:69:THR:C	1:B:71:ASP:H	2.27	0.42
1:C:15:THR:O	1:C:23:TRP:NE1	2.52	0.42
1:C:285:THR:HB	4:C:548:HOH:O	2.18	0.42
1:A:64:TRP:CZ3	1:A:77:VAL:HG22	2.54	0.42
1:B:120:PHE:CE1	1:B:124:ALA:HB2	2.54	0.42
1:B:59:LEU:O	1:B:60:ALA:C	2.63	0.42
1:A:324:ARG:HH11	1:A:324:ARG:CG	2.33	0.41
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.87	0.41
1:C:142:PHE:HA	1:C:145:ILE:HG22	2.03	0.41
1:B:19:SER:N	1:B:20:PRO:CD	2.84	0.41
1:B:34:ARG:O	1:B:35:LEU:C	2.64	0.40
1:B:56:SER:HA	1:B:64:TRP:O	2.21	0.40
1:C:132:LEU:HD22	1:C:256:LEU:HG	2.01	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	313/318 (98%)	300 (96%)	11 (4%)	2 (1%)	22	21
1	B	314/318 (99%)	280 (89%)	26 (8%)	8 (2%)	4	2
1	C	311/318 (98%)	294 (94%)	16 (5%)	1 (0%)	37	41
All	All	938/954 (98%)	874 (93%)	53 (6%)	11 (1%)	11	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	B	85	VAL
1	B	287	GLN
1	B	291	PRO
1	C	19	SER
1	A	81	ASP
1	B	286	SER
1	B	52	PRO
1	B	288	ALA
1	B	289	LYS
1	B	190	PRO

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	264/266 (99%)	250 (95%)	14 (5%)	19	19
1	B	265/266 (100%)	247 (93%)	18 (7%)	13	11
1	C	263/266 (99%)	253 (96%)	10 (4%)	28	34
All	All	792/798 (99%)	750 (95%)	42 (5%)	19	19

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	11	MET
1	A	19	SER
1	A	58	VAL
1	A	77	VAL
1	A	79	ARG
1	A	83	SER
1	A	91	GLU
1	A	111	SER
1	A	125	GLN
1	A	216	LEU
1	A	238	LYS

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Mol	Chain	Res	Type
1	A	271	VAL
1	A	315	GLN
1	B	11	MET
1	B	13	HIS
1	B	30	ARG
1	B	52	PRO
1	B	67	THR
1	B	71	ASP
1	B	77	VAL
1	B	78	TYR
1	B	82	ASP
1	B	91	GLU
1	B	95	THR
1	B	118	SER
1	B	141	LEU
1	B	171	ILE
1	B	194	THR
1	B	227	GLN
1	B	292	SER
1	B	315	GLN
1	C	121	GLN
1	C	122	ARG
1	C	141	LEU
1	C	145	ILE
1	C	197	ARG
1	C	201	LEU
1	C	216	LEU
1	C	219	GLN
1	C	225	LEU
1	C	289	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	50	GLN
1	A	68	GLN
1	A	112	HIS
1	A	119	HIS
1	A	226	GLN
1	B	54	HIS
1	B	112	HIS

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Mol	Chain	Res	Type
1	B	135	GLN
1	B	149	ASN
1	B	219	GLN
1	C	50	GLN
1	C	68	GLN
1	C	119	HIS
1	C	219	GLN
1	C	287	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
2	A1IEJ	B	401	-	17,20,20	0.80	1 (5%)	20,27,27	1.08	2 (10%)
2	A1IEJ	A	401	-	17,20,20	0.75	0	20,27,27	1.03	2 (10%)
2	A1IEJ	C	401	-	17,20,20	0.67	0	20,27,27	1.07	2 (10%)

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	A1IEJ	B	401	-	-	0/7/7/7	0/3/3/3
2	A1IEJ	A	401	-	-	0/7/7/7	0/3/3/3
2	A1IEJ	C	401	-	-	0/7/7/7	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1IEJ	C5-C4	-2.16	1.46	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	A1IEJ	C4-N3-C10	2.60	109.24	103.90
2	B	401	A1IEJ	C4-N3-C10	2.55	109.13	103.90
2	A	401	A1IEJ	C4-N3-C10	2.45	108.94	103.90
2	B	401	A1IEJ	C12-C11-C10	-2.13	117.02	120.08
2	A	401	A1IEJ	C2-C3-C4	2.09	129.75	127.48
2	C	401	A1IEJ	C12-C11-C10	-2.02	117.18	120.08

There are no chirality outliers.

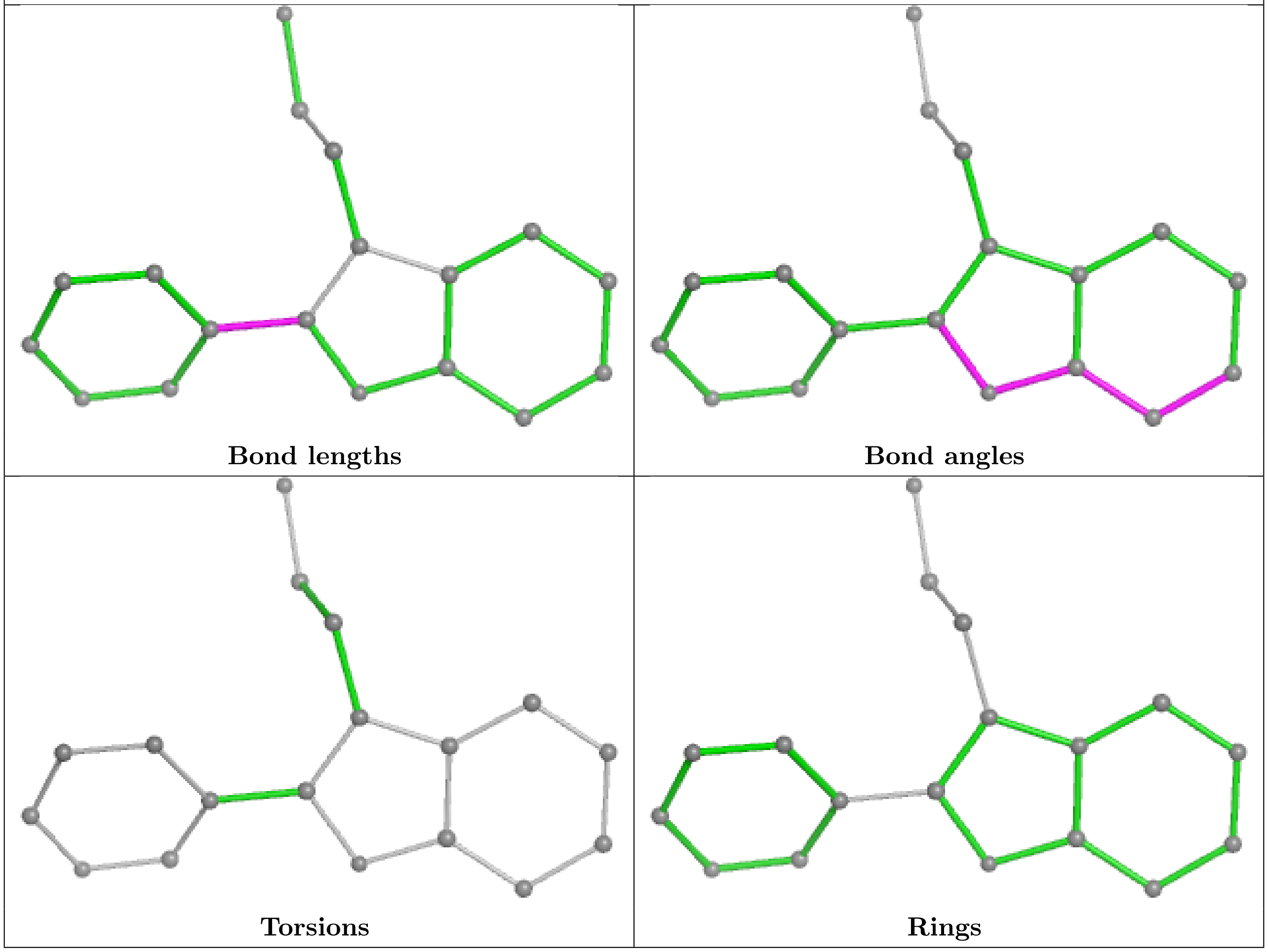
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 A1IEJ B 401



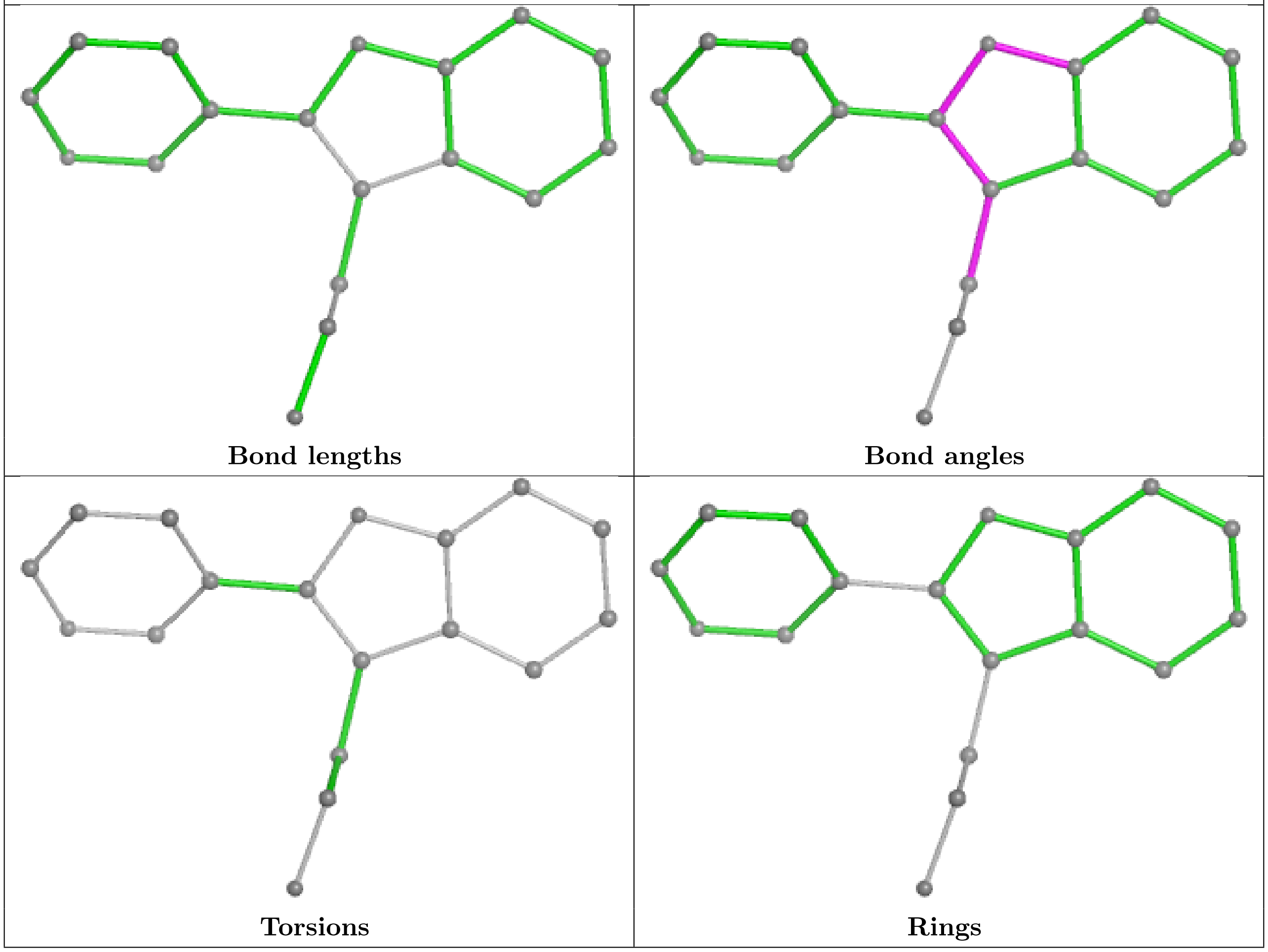
Bond lengths

Bond angles

Torsions

Rings

Ligand A1IEJ A 401

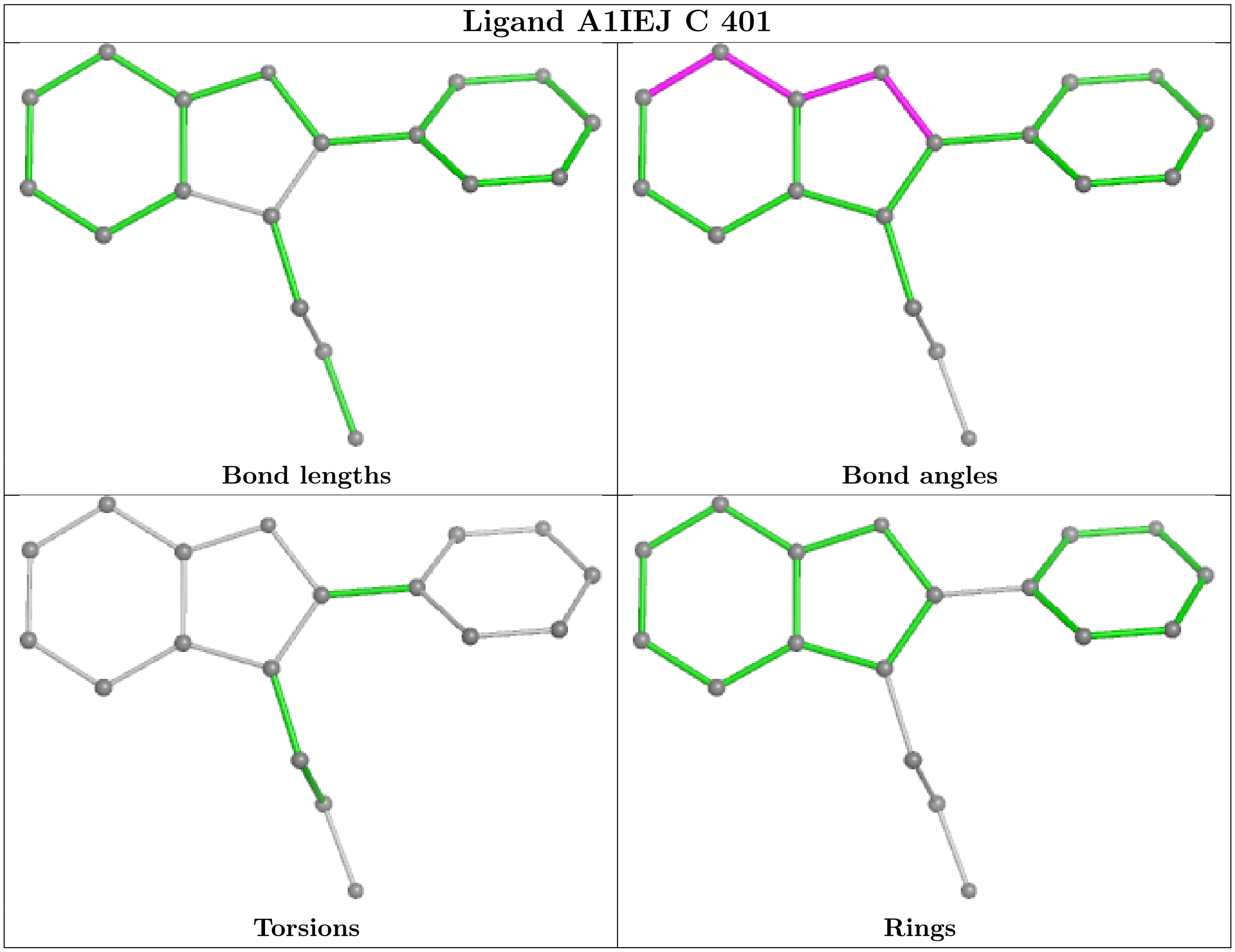


Bond lengths

Bond angles

Torsions

Rings



5.7 Other polymers

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^{th} 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	315/318 (99%)	-0.45	8 (2%)	58	59	27, 41, 80, 145	0
1	B	316/318 (99%)	0.34	24 (7%)	21	20	33, 59, 110, 164	0
1	C	315/318 (99%)	0.26	17 (5%)	32	32	32, 61, 100, 151	0
All	All	946/954 (99%)	0.05	49 (5%)	34	34	27, 54, 102, 164	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	4.0
1	B	74	TYR	3.9
1	B	22	LEU	3.8
1	C	85	VAL	3.8
1	B	87	ARG	3.8
1	C	288	ALA	3.7
1	A	288	ALA	3.7
1	C	324	ARG	3.5
1	A	10	HIS	3.4
1	C	289	LYS	3.4
1	A	81	ASP	3.2
1	C	16	LEU	3.2
1	B	93	LEU	3.1
1	B	19	SER	3.1
1	C	146	CYS	3.0
1	B	289	LYS	2.9
1	C	90	LEU	2.9
1	C	145	ILE	2.9
1	B	85	VAL	2.9
1	C	80	GLY	2.9
1	B	48	LYS	2.8
1	B	285	THR	2.8
1	C	82	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	26	ILE	2.6
1	B	81	ASP	2.6
1	C	149	ASN	2.6
1	B	10	HIS	2.5
1	C	81	ASP	2.5
1	B	86	SER	2.5
1	A	61	ASP	2.4
1	B	324	ARG	2.4
1	A	285	THR	2.3
1	C	17	SER	2.3
1	C	18	SER	2.3
1	B	23	TRP	2.3
1	C	294	LEU	2.3
1	A	324	ARG	2.2
1	B	88	PRO	2.2
1	C	147	SER	2.2
1	A	83	SER	2.2
1	B	17	SER	2.1
1	B	80	GLY	2.1
1	B	11	MET	2.1
1	A	286	SER	2.1
1	C	150	ASN	2.1
1	B	69	THR	2.1
1	B	16	LEU	2.1
1	B	171	ILE	2.0
1	B	52	PRO	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)

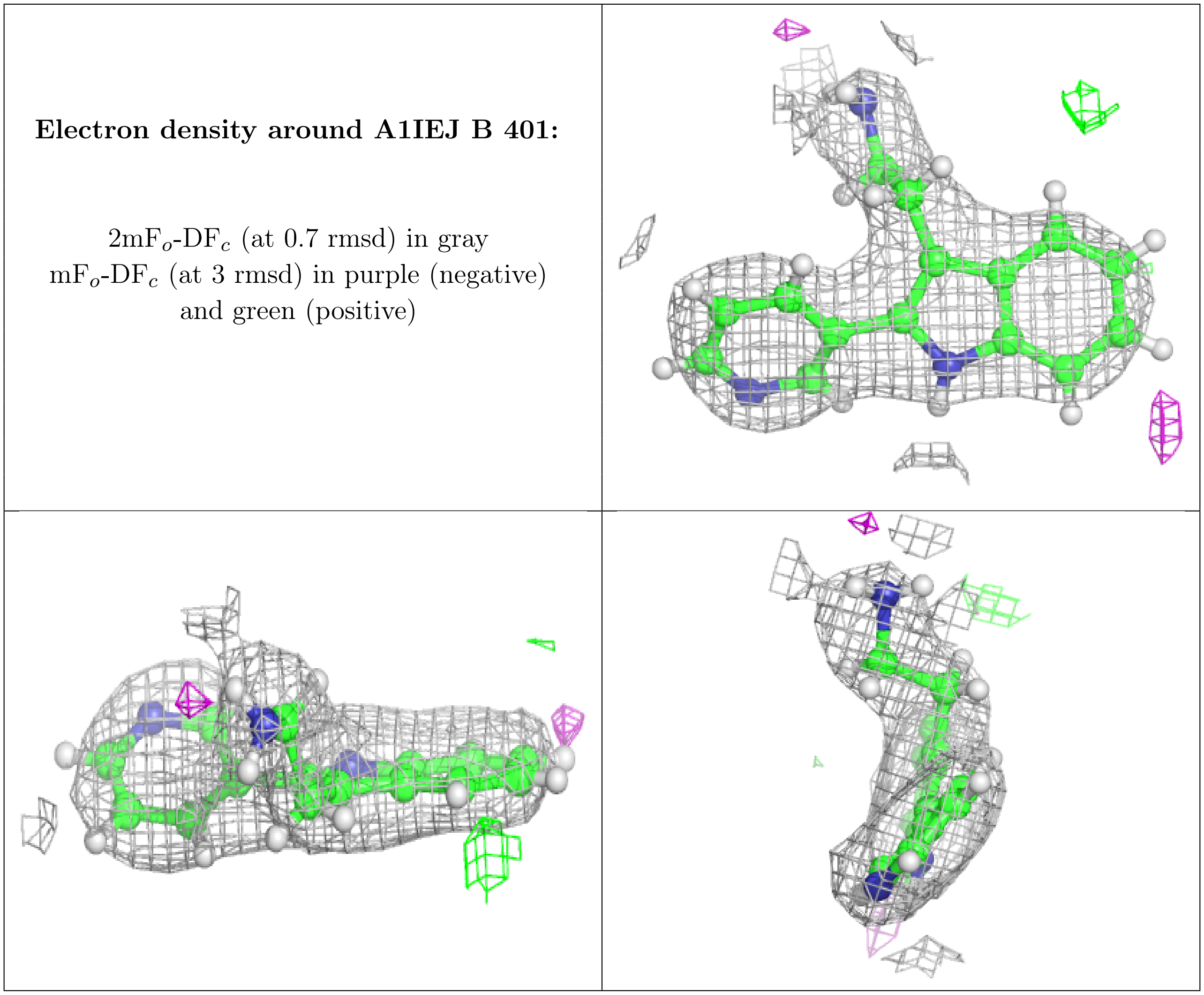
There are no oligosaccharides in this entry.

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($Å^2$)	Q<0.9
2	A1IEJ	B	401	18/18	0.96	0.07	37,42,49,52	0
2	A1IEJ	C	401	18/18	0.96	0.07	43,49,62,69	0
2	A1IEJ	A	401	18/18	0.97	0.05	30,37,41,43	0
3	NI	A	402	1/1	1.00	0.03	36,36,36,36	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.

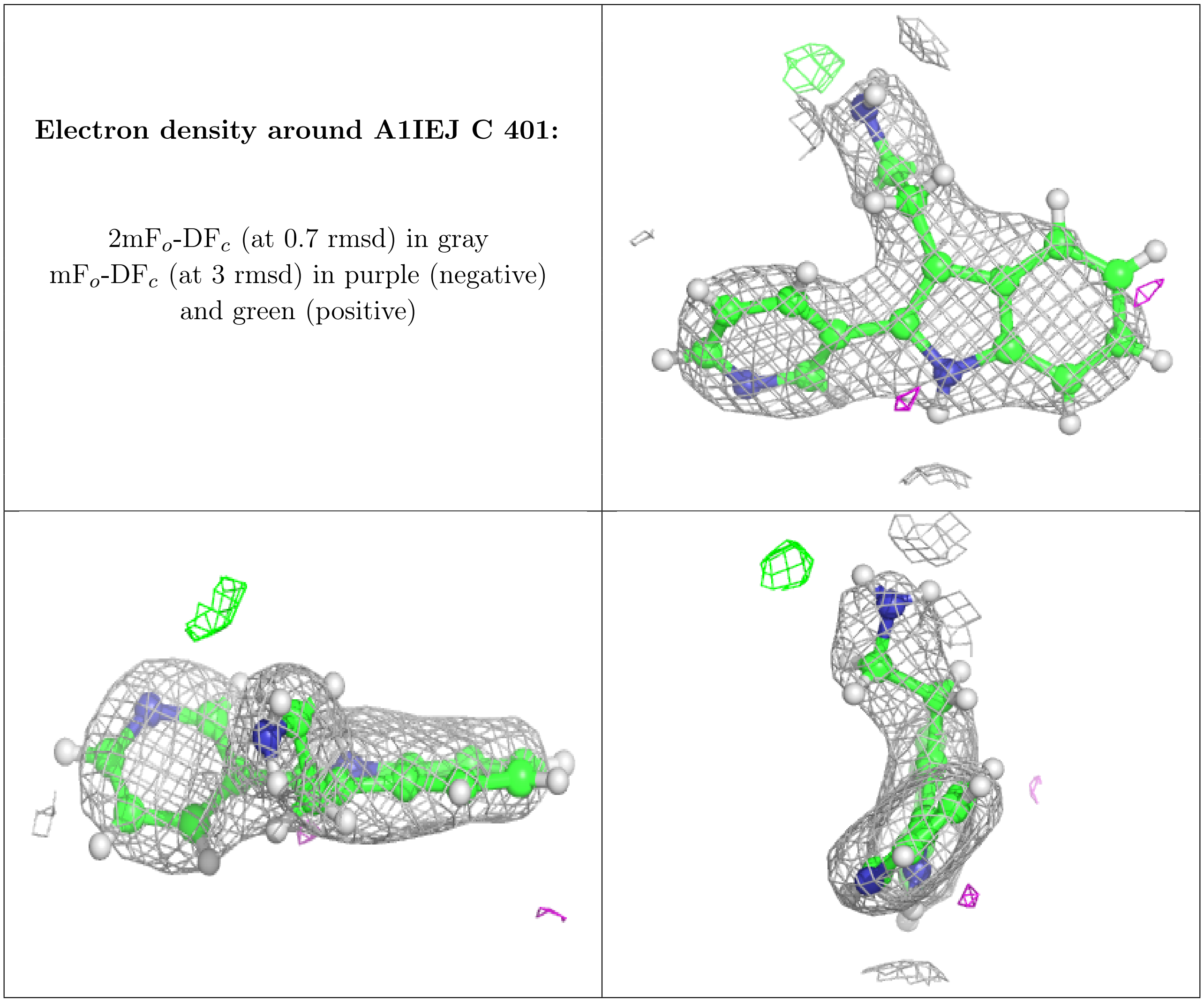


Electron density around A1IEJ B 401:

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

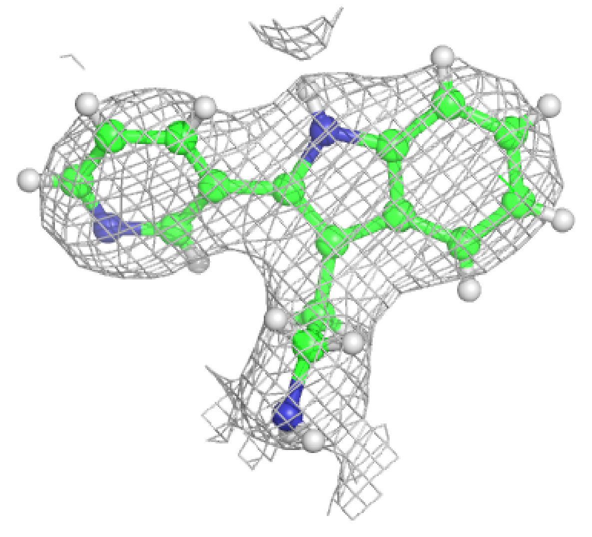
Electron density around A1IEJ C 401:

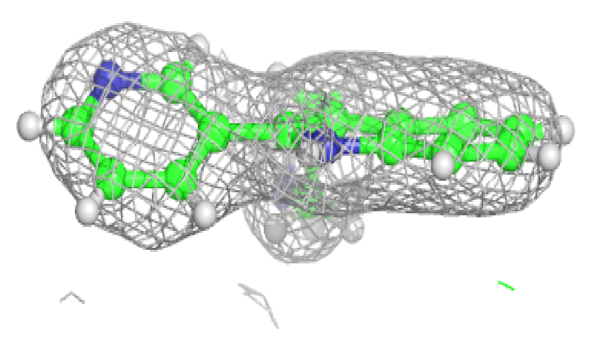
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

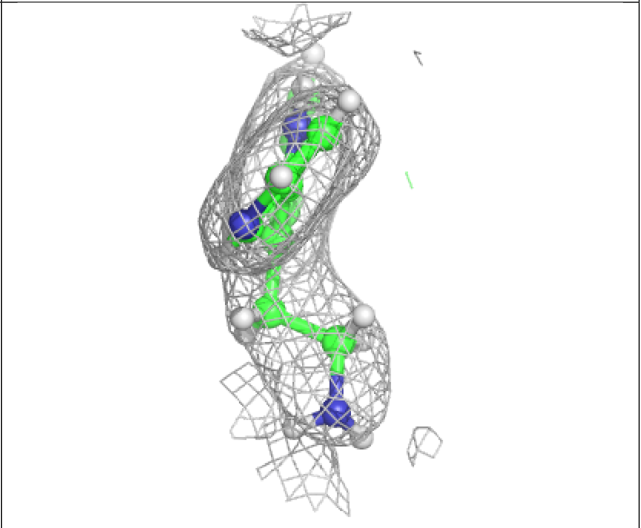


Electron density around A1IEJ A 401:

$2mF_o$-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 ⓘ

There are no such residues in this entry.