



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:23 AM UTC

PDB ID : 4E73 / pdb\_00004e73  
Title : Crystal structure of JNK1beta-JIP in complex with an azaquinolone inhibitor  
Authors : Lukacs, C.M.; Janson, C.A.  
Deposited on : 2012-03-16  
Resolution : 2.27 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 : 4-5-2 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

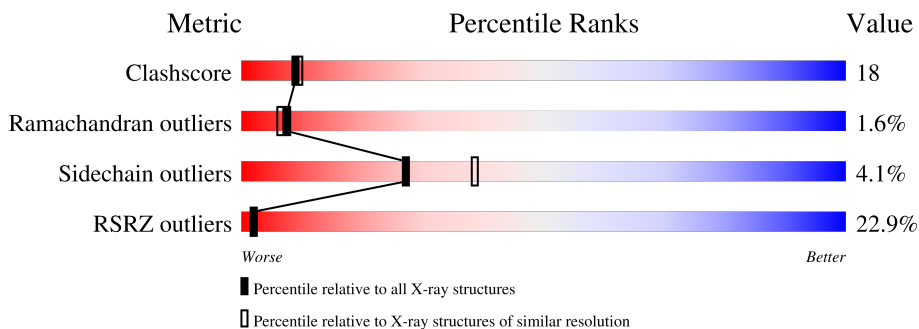
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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  $\geq 3$ , 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	369	
2	B	11	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2784 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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2581	1659	435	467	20	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	HIS	-	expression tag	UNP P45983
A	365	HIS	-	expression tag	UNP P45983
A	366	HIS	-	expression tag	UNP P45983
A	367	HIS	-	expression tag	UNP P45983
A	368	HIS	-	expression tag	UNP P45983
A	369	HIS	-	expression tag	UNP P45983

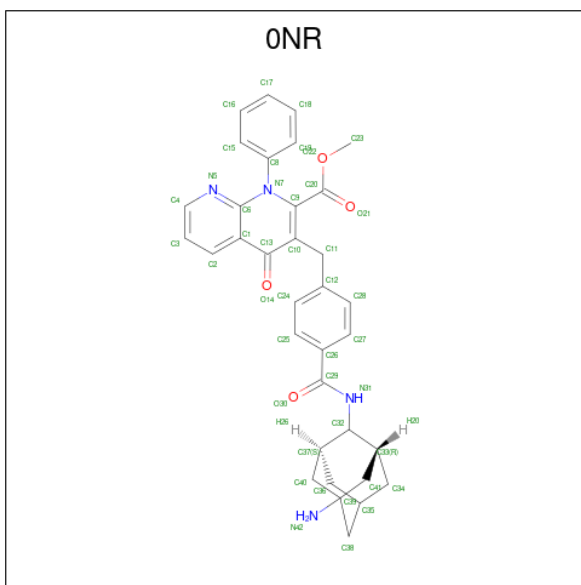
- Molecule 2 is a protein called C-Jun-amino-terminal kinase-interacting protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	72	46	14	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	153	LYS	ARG	conflict	UNP Q9UQF2

- Molecule 3 is methyl 3-(4-{{(1R,2S,3S,5S,7s)-5-aminotricyclo[3.3.1.1<sup>3,7</sup>]dec-2-yl}carbamoyl}benzyl)-4-oxo-1-phenyl-1,4-dihydro-1,8-naphthyridine-2-carboxylate (CCD ID: 0NR) (formula: C<sub>34</sub>H<sub>34</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	42	34	4	4	0	0

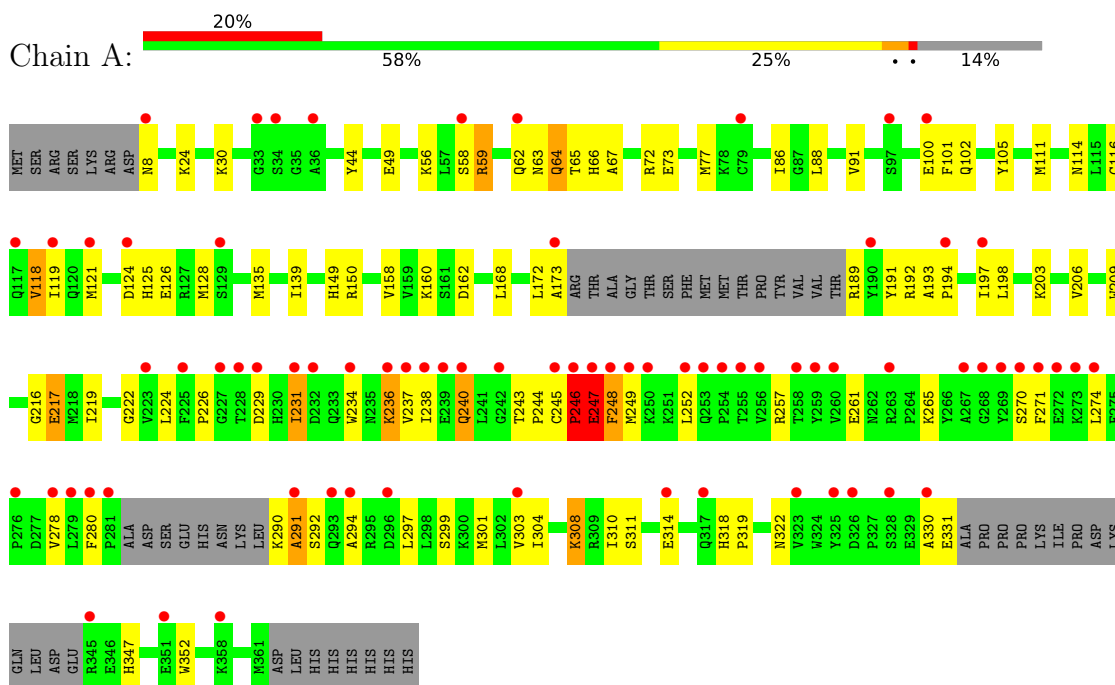
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	88	88	88	0	0
4	B	1	1	1	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mitogen-activated protein kinase 8



- Molecule 2: C-Jun-amino-terminal kinase-interacting protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.90Å 79.84Å 85.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.70 – 2.27 27.70 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.70-2.27) 99.0 (27.70-2.27)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.26Å)	Xtrriage
Refinement program	CNX 2005	Depositor
R, $R_{free}$	0.247 , 0.282 0.248 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: 0NR

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	0.40	0/2635	0.73	0/3555
2	B	0.35	0/73	0.76	0/98
All	All	0.40	0/2708	0.73	0/3653

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	PRO	Peptide

### 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	2581	0	2601	100	0
2	B	72	0	82	4	0
3	A	42	0	34	0	0
4	A	88	0	0	4	0
4	B	1	0	0	0	0
All	All	2784	0	2717	100	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 18.

All (100) 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:59:ARG:HB3	1:A:59:ARG:NH1	1.83	0.94
1:A:245:CYS:HB2	1:A:246:PRO:HD2	1.53	0.90
1:A:245:CYS:SG	1:A:247:GLU:HB3	2.14	0.88
1:A:231:ILE:H	1:A:231:ILE:HD13	1.42	0.84
1:A:63:ASN:HD22	1:A:65:THR:H	1.24	0.83
1:A:119:ILE:HD11	1:A:217:GLU:HB3	1.61	0.81
1:A:189:ARG:HD3	1:A:197:ILE:HG22	1.64	0.80
1:A:59:ARG:HB3	1:A:59:ARG:HH11	1.50	0.77
1:A:297:LEU:HD11	1:A:301:MET:HE3	1.70	0.73
1:A:240:GLN:NE2	1:A:274:LEU:HD22	2.08	0.69
1:A:59:ARG:HB2	1:A:62:GLN:HB2	1.73	0.68
1:A:226:PRO:HD2	1:A:236:LYS:HD3	1.77	0.67
1:A:249:MET:O	1:A:257:ARG:HD2	1.95	0.67
1:A:216:GLY:HA3	1:A:224:LEU:HD11	1.77	0.66
1:A:63:ASN:ND2	1:A:65:THR:H	1.94	0.65
1:A:271:PHE:CZ	1:A:299:SER:HA	2.31	0.64
1:A:290:LYS:O	1:A:292:SER:N	2.31	0.64
1:A:58:SER:C	1:A:59:ARG:HG2	2.22	0.64
1:A:249:MET:HA	1:A:252:LEU:HD12	1.81	0.62
1:A:118:VAL:O	1:A:121:MET:HG2	1.99	0.62
1:A:197:ILE:HG13	1:A:198:LEU:CD1	2.28	0.62
1:A:189:ARG:HG2	1:A:192:ARG:HD2	1.80	0.62
1:A:247:GLU:O	1:A:248:PHE:HB2	2.00	0.61
1:A:197:ILE:HG13	1:A:198:LEU:HD12	1.82	0.61
1:A:121:MET:HE1	2:B:161:ASN:HB3	1.82	0.60
1:A:160:LYS:HB3	1:A:162:ASP:OD1	2.01	0.60
1:A:322:ASN:HB2	4:A:581:HOH:O	2.03	0.59
1:A:297:LEU:CD1	1:A:301:MET:HE3	2.33	0.59
1:A:56:LYS:HE3	1:A:105:TYR:OH	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135[A]:MET:O	1:A:139:ILE:HG13	2.03	0.58
1:A:319:PRO:HA	1:A:322:ASN:HD21	1.69	0.57
1:A:194:PRO:O	1:A:198:LEU:HD13	2.04	0.57
1:A:73:GLU:O	1:A:77:MET:HG3	2.04	0.57
1:A:67:ALA:HB1	1:A:352:TRP:HB3	1.87	0.57
1:A:118:VAL:HG21	2:B:160:LEU:HD21	1.85	0.56
1:A:319:PRO:HA	1:A:322:ASN:ND2	2.21	0.56
1:A:59:ARG:HB3	1:A:59:ARG:CZ	2.36	0.56
1:A:172:LEU:O	1:A:173:ALA:CB	2.54	0.55
1:A:63:ASN:HD22	1:A:65:THR:N	2.01	0.55
1:A:244:PRO:O	1:A:249:MET:HE2	2.07	0.55
1:A:249:MET:HA	1:A:252:LEU:CD1	2.37	0.55
1:A:257:ARG:O	1:A:261:GLU:HB2	2.08	0.53
1:A:135[B]:MET:O	1:A:139:ILE:HG13	2.09	0.53
1:A:63:ASN:HD21	1:A:65:THR:HB	1.73	0.53
1:A:116:CYS:O	1:A:119:ILE:HG22	2.08	0.53
1:A:126:GLU:HG2	2:B:157:PRO:HG3	1.90	0.52
1:A:198:LEU:HD11	1:A:234:TRP:CE3	2.45	0.52
1:A:111:MET:HG3	1:A:158:VAL:HG23	1.93	0.51
1:A:100:GLU:O	1:A:102:GLN:HG2	2.10	0.50
1:A:59:ARG:HG3	1:A:66:HIS:CE1	2.46	0.49
1:A:270:SER:O	1:A:274:LEU:HG	2.12	0.49
1:A:203:LYS:O	1:A:206:VAL:HG12	2.12	0.49
1:A:172:LEU:O	1:A:173:ALA:HB3	2.13	0.48
1:A:234:TRP:O	1:A:238:ILE:HG12	2.12	0.48
1:A:310:ILE:HG12	1:A:311:SER:N	2.28	0.48
1:A:247:GLU:O	1:A:248:PHE:CB	2.62	0.48
1:A:229:ASP:HB3	1:A:231:ILE:HD11	1.96	0.47
1:A:231:ILE:H	1:A:231:ILE:CD1	2.11	0.47
1:A:330:ALA:O	1:A:331:GLU:HG3	2.14	0.47
1:A:318:HIS:CG	1:A:319:PRO:HD2	2.50	0.47
1:A:297:LEU:CG	1:A:301:MET:HE3	2.45	0.46
1:A:246:PRO:O	1:A:248:PHE:N	2.49	0.46
1:A:72:ARG:HD3	4:A:583:HOH:O	2.16	0.46
1:A:124:ASP:O	1:A:128:MET:HB2	2.15	0.46
1:A:72:ARG:NE	4:A:588:HOH:O	2.26	0.46
1:A:119:ILE:CD1	1:A:217:GLU:HB3	2.38	0.45
1:A:189:ARG:CG	1:A:192:ARG:HD2	2.45	0.45
1:A:245:CYS:HB2	1:A:246:PRO:CD	2.33	0.45
1:A:149:HIS:O	1:A:150:ARG:HB2	2.16	0.45
1:A:72:ARG:CZ	1:A:173:ALA:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG12	1:A:304:ILE:HD11	1.98	0.44
1:A:231:ILE:HD13	1:A:231:ILE:N	2.23	0.44
1:A:229:ASP:HB3	1:A:231:ILE:CD1	2.48	0.44
1:A:125:HIS:CD2	1:A:290:LYS:HB2	2.53	0.44
1:A:63:ASN:ND2	1:A:65:THR:N	2.64	0.43
1:A:189:ARG:NH1	1:A:192:ARG:HH11	2.15	0.43
1:A:193:ALA:HA	1:A:209:TRP:CD1	2.54	0.43
1:A:310:ILE:HD11	1:A:314:GLU:HB3	2.01	0.43
1:A:240:GLN:HE21	1:A:240:GLN:HB3	1.52	0.43
1:A:126:GLU:HG2	2:B:157:PRO:CG	2.49	0.42
1:A:44:TYR:OH	1:A:49:GLU:HA	2.19	0.42
1:A:8:ASN:O	1:A:24:LYS:HE3	2.19	0.42
1:A:58:SER:O	1:A:59:ARG:C	2.62	0.42
1:A:219:ILE:HD13	1:A:280:PHE:CZ	2.55	0.42
1:A:280:PHE:CD1	1:A:291:ALA:HA	2.54	0.42
1:A:86:ILE:HG13	1:A:168:LEU:HD12	2.03	0.41
1:A:88:LEU:HD11	1:A:91:VAL:CG2	2.50	0.41
1:A:114:ASN:OD1	1:A:114:ASN:C	2.63	0.41
1:A:280:PHE:HE1	1:A:294:ALA:HB3	1.86	0.41
1:A:189:ARG:CD	1:A:197:ILE:HG22	2.43	0.41
1:A:64:GLN:NE2	1:A:347:HIS:O	2.53	0.41
1:A:280:PHE:CE1	1:A:294:ALA:HB3	2.56	0.41
1:A:191:TYR:OH	1:A:217:GLU:OE1	2.26	0.41
1:A:100:GLU:O	1:A:101:PHE:C	2.63	0.41
1:A:303:VAL:HG11	1:A:308:LYS:HB2	2.03	0.41
1:A:245:CYS:CB	1:A:246:PRO:HD2	2.33	0.40
1:A:203:LYS:NZ	4:A:586:HOH:O	2.53	0.40
1:A:217:GLU:HG2	1:A:222:GLY:C	2.47	0.40
1:A:243:THR:HG22	1:A:244:PRO:O	2.22	0.40
1:A:88:LEU:HD11	1:A:91:VAL:HG22	2.03	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	311/369 (84%)	293 (94%)	14 (4%)	4 (1%)	9	9
2	B	7/11 (64%)	6 (86%)	0	1 (14%)	0	0
All	All	318/380 (84%)	299 (94%)	14 (4%)	5 (2%)	7	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	PHE
1	A	291	ALA
2	B	155	LYS
1	A	246	PRO
1	A	247	GLU

### 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	285/331 (86%)	273 (96%)	12 (4%)	26	37
2	B	9/11 (82%)	9 (100%)	0	100	100
All	All	294/342 (86%)	282 (96%)	12 (4%)	27	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	59	ARG
1	A	64	GLN
1	A	118	VAL
1	A	217	GLU
1	A	231	ILE
1	A	236	LYS
1	A	240	GLN

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	265	LYS
1	A	278	VAL
1	A	308	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	27	GLN
1	A	28	ASN
1	A	62	GLN
1	A	63	ASN
1	A	90	ASN
1	A	102	GLN
1	A	141	HIS
1	A	240	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	0NR	A	401	-	48,48,48	2.01	23 (47%)	62,72,72	2.10	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0NR	A	401	-	-	1/22/53/53	0/8/7/7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	0NR	C11-C10	3.58	1.56	1.51
3	A	401	0NR	C9-N7	3.45	1.45	1.40
3	A	401	0NR	C6-N7	3.29	1.45	1.40
3	A	401	0NR	C27-C26	2.91	1.43	1.39
3	A	401	0NR	C6-N5	2.82	1.39	1.34
3	A	401	0NR	C28-C27	2.75	1.43	1.38
3	A	401	0NR	C19-C8	2.75	1.44	1.39
3	A	401	0NR	C15-C8	2.70	1.44	1.39
3	A	401	0NR	C41-C39	2.60	1.58	1.53
3	A	401	0NR	C3-C2	2.53	1.43	1.38
3	A	401	0NR	C2-C1	2.51	1.43	1.39
3	A	401	0NR	C38-C39	2.43	1.57	1.53
3	A	401	0NR	C28-C12	2.40	1.43	1.38
3	A	401	0NR	C40-C39	2.33	1.57	1.53
3	A	401	0NR	C25-C26	2.31	1.42	1.39
3	A	401	0NR	C24-C12	2.21	1.43	1.38
3	A	401	0NR	C18-C17	2.19	1.43	1.38
3	A	401	0NR	C29-N31	2.19	1.39	1.34
3	A	401	0NR	C39-N42	-2.14	1.42	1.49
3	A	401	0NR	C10-C13	2.11	1.52	1.47
3	A	401	0NR	C33-C32	2.06	1.58	1.53
3	A	401	0NR	C34-C33	2.05	1.58	1.53
3	A	401	0NR	C4-N5	2.02	1.38	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	0NR	C11-C10-C9	11.50	128.77	116.79
3	A	401	0NR	C20-C9-C10	-8.88	115.76	122.63
3	A	401	0NR	C12-C11-C10	-2.82	108.75	114.24
3	A	401	0NR	C4-N5-C6	2.43	120.55	115.05
3	A	401	0NR	C6-C1-C13	-2.38	120.17	121.88
3	A	401	0NR	C20-C9-N7	2.33	118.74	114.05
3	A	401	0NR	O22-C20-O21	2.29	127.87	123.50
3	A	401	0NR	N5-C6-N7	2.13	120.40	117.52

There are no chirality outliers.

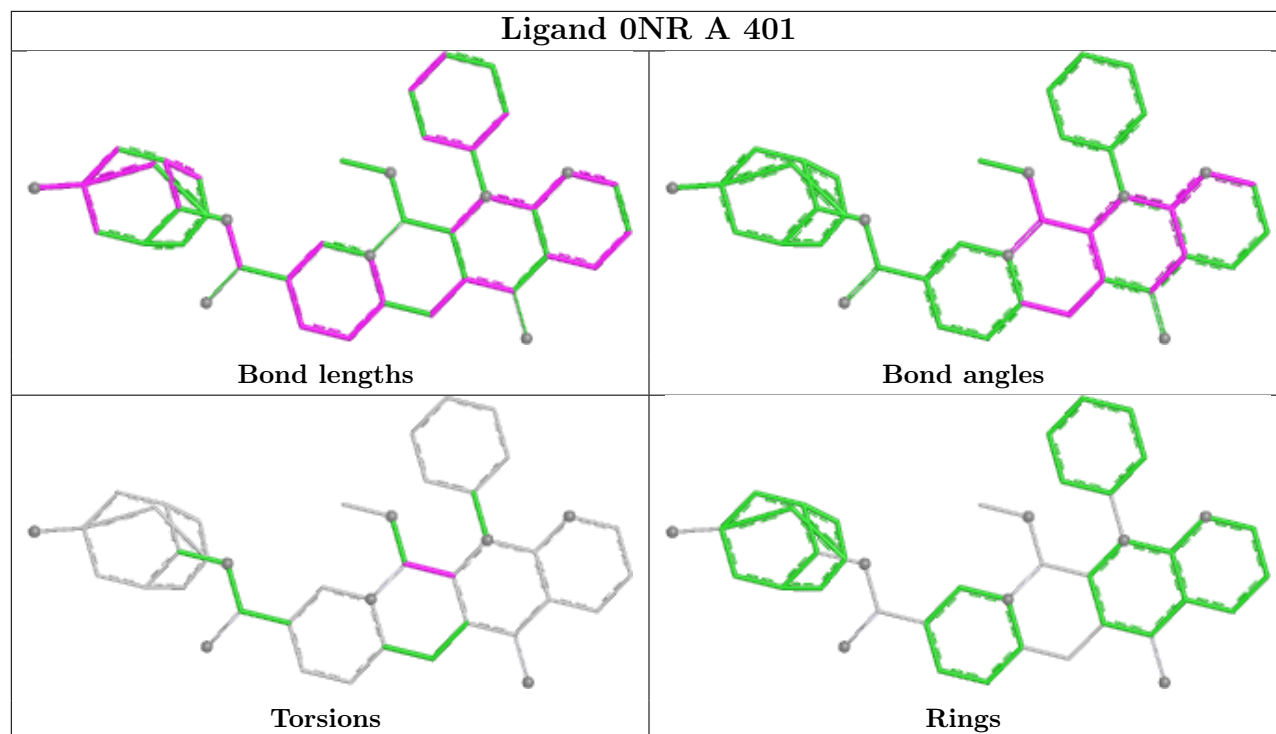
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	0NR	O21-C20-C9-C10

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	318/369 (86%)	1.21	75 (23%) <b>2</b>   <b>2</b>	20, 56, 99, 113	1 (0%)
2	B	9/11 (81%)	1.42	0 <b>100</b>   <b>100</b>	66, 67, 80, 82	0
All	All	327/380 (86%)	1.22	75 (22%) <b>2</b>   <b>2</b>	20, 56, 99, 113	1 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	CYS	5.0
1	A	256	VAL	4.8
1	A	254	PRO	4.7
1	A	326	ASP	4.6
1	A	258	THR	4.1
1	A	291	ALA	4.1
1	A	227	GLY	4.1
1	A	242	GLY	3.9
1	A	273	LYS	3.9
1	A	276	PRO	3.8
1	A	238	ILE	3.8
1	A	260	VAL	3.8
1	A	278	VAL	3.7
1	A	259	TYR	3.6
1	A	231	ILE	3.5
1	A	294	ALA	3.5
1	A	229	ASP	3.4
1	A	274	LEU	3.4
1	A	268	GLY	3.4
1	A	119	ILE	3.3
1	A	314	GLU	3.3
1	A	58	SER	3.3
1	A	34	SER	3.2
1	A	248	PHE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	236	LYS	3.2
1	A	173	ALA	2.9
1	A	228	THR	2.9
1	A	281	PRO	2.9
1	A	323	VAL	2.9
1	A	246	PRO	2.9
1	A	117	GLN	2.9
1	A	245	CYS	2.9
1	A	317	GLN	2.9
1	A	239	GLU	2.9
1	A	303	VAL	2.8
1	A	279	LEU	2.8
1	A	8	ASN	2.7
1	A	97	SER	2.7
1	A	270	SER	2.7
1	A	328	SER	2.7
1	A	36	ALA	2.6
1	A	234	TRP	2.6
1	A	240	GLN	2.6
1	A	253	GLN	2.6
1	A	197	ILE	2.5
1	A	62	GLN	2.5
1	A	263	ARG	2.5
1	A	345	ARG	2.5
1	A	190	TYR	2.4
1	A	255	THR	2.4
1	A	129	SER	2.4
1	A	237	VAL	2.4
1	A	280	PHE	2.4
1	A	100	GLU	2.4
1	A	124	ASP	2.3
1	A	194	PRO	2.3
1	A	267	ALA	2.3
1	A	121	MET	2.3
1	A	223	VAL	2.3
1	A	271	PHE	2.3
1	A	33	GLY	2.3
1	A	247	GLU	2.2
1	A	252	LEU	2.2
1	A	250	LYS	2.2
1	A	325	TYR	2.2
1	A	225	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	330	ALA	2.1
1	A	249	MET	2.1
1	A	269	TYR	2.1
1	A	272	GLU	2.1
1	A	358	LYS	2.0
1	A	351	GLU	2.0
1	A	293	GLN	2.0
1	A	232	ASP	2.0
1	A	296	ASP	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](#)

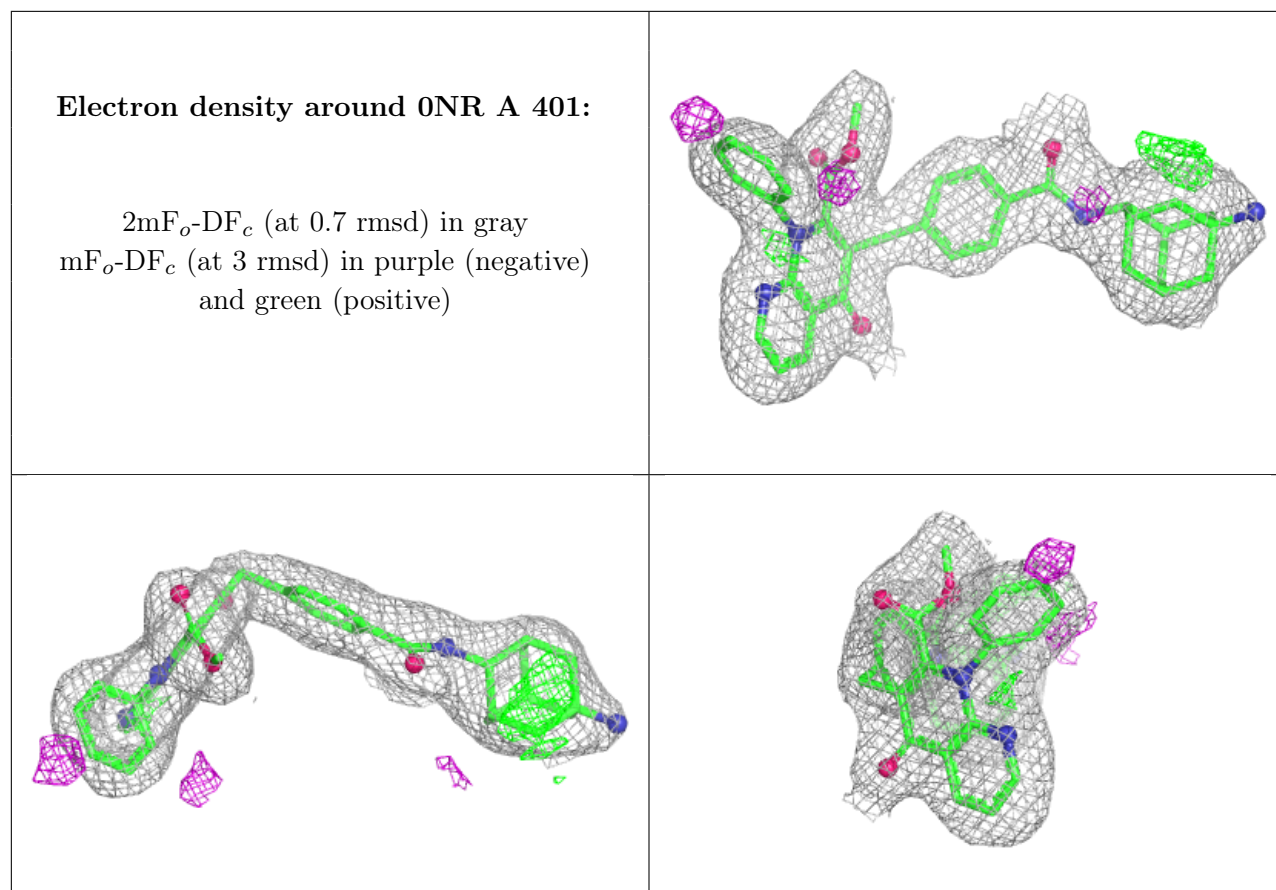
There are no oligosaccharides in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
3	ONR	A	401	42/42	0.92	0.11	24,39,63,63	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.