

# Full wwPDB X-ray Structure Validation Report (i)

#### May 24, 2022 - 10:18 am BST

PDB ID	:	7AYZ
Title	:	Structure of the mouse 8-oxoguanine DNA Glycosylase mOGG1 in complex
		with activator TH10785
Authors	:	Masuyer, G.; Davies, J.R.; Stenmark, P.
Deposited on	:	2020-11-13
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

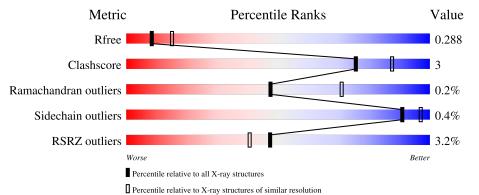
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4	:::::::::::::::::::::::::::::::::::::::	<ul> <li>1.8.4, CSD as541be (2020)</li> <li>1.13</li> <li>2.28.1</li> <li>1.1.7 (2018)</li> <li>20191225.v01 (using entries in the PDB archive December 25th 2019)</li> <li>5.8.0267</li> <li>7.1.010 (Gargrove)</li> </ul>
CCP4 Ideal geometry (proteins)		
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	e ( )
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# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.60 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
$R_{free}$	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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	AAA	318	% • 92%	6%	·
1	BBB	318	4% 87%	11%	·
1	CCC	318	90%	8%	·



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7509 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	AAA	311	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	AAA	311	2484	1581	448	444	11	0	0	0
1	BBB	310	Total	С	Ν	0	S	0	0	0
	DDD	510	2472	1573	446	442	11	0	0	U
1	CCC	313	Total	С	Ν	0	S	0	0	0
	515	2425	1540	433	441	11	0	0	0	

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

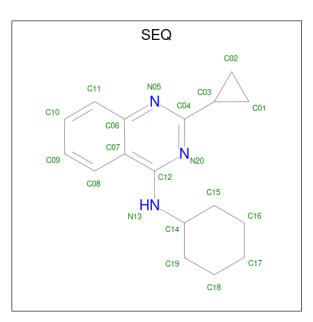
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	8	GLY	-	expression tag	UNP 008760
AAA	10	HIS	SER	conflict	UNP 008760
BBB	8	GLY	-	expression tag	UNP 008760
BBB	10	HIS	SER	conflict	UNP 008760
CCC	8	GLY	-	expression tag	UNP 008760
CCC	10	HIS	SER	conflict	UNP 008760

• Molecule 2 is {N}-cyclohexyl-2-cyclopropyl-quinazolin-4-amine (three-letter code: SEQ) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).







Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total         C         N           20         17         3	0	0
2	BBB	1	Total         C         N           20         17         3	0	0
2	CCC	1	Total         C         N           20         17         3	0	0

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	sidues Atoms		AltConf
3	AAA	1	Total Ni 1 1	0	0

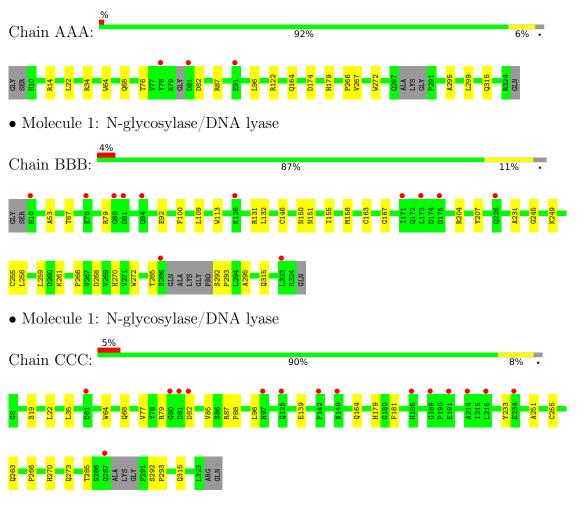
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	30	Total         O           30         30	0	0
4	BBB	24	Total O 24 24	0	0
4	CCC	13	Total O 13 13	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: N-glycosylase/DNA lyase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	99.9(73.87-2.60)	Depositor
(in resolution range)	99.9 (73.76-2.60)	EDS
R <sub>merge</sub>	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.12 (at 2.62 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
$R, R_{free}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
$R_{free}$ test set	1850 reflections $(5.20\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	65.5	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7509	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: SEQ, NI

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	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	AAA	0.63	0/2553	0.71	0/3473	
1	BBB	0.64	0/2541	0.72	0/3458	
1	CCC	0.66	0/2493	0.71	0/3401	
All	All	0.64	0/7587	0.72	0/10332	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (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	AAA	2484	0	2427	11	0
1	BBB	2472	0	2415	21	0
1	CCC	2425	0	2309	14	0
2	AAA	20	0	0	0	0
2	BBB	20	0	0	0	0
2	$\operatorname{CCC}$	20	0	0	0	0
3	AAA	1	0	0	0	0
4	AAA	30	0	0	0	0
4	BBB	24	0	0	0	0
4	CCC	13	0	0	0	0
All	All	7509	0	7151	45	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 3.

All (45) 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:AAA:266:PRO:HD2	1:AAA:315:GLN:NE2	2.04	0.72
1:CCC:266:PRO:HD2	1:CCC:315:GLN:HE22	1.54	0.72
1:AAA:22:LEU:HA	1:AAA:87:ARG:HG2	1.74	0.69
1:BBB:266:PRO:HD2	1:BBB:315:GLN:HE22	1.56	0.69
1:CCC:64:TRP:CZ3	1:CCC:96:LEU:HD11	2.28	0.68
1:BBB:163:CYS:O	1:BBB:167:GLY:N	2.26	0.67
1:CCC:77:VAL:HG23	1:CCC:88:PRO:HG3	1.78	0.64
1:AAA:266:PRO:HD2	1:AAA:315:GLN:HE22	1.64	0.62
1:CCC:22:LEU:HD21	1:CCC:85:VAL:HG12	1.83	0.60
1:BBB:150:ASN:HD21	1:BBB:158:MET:CE	2.18	0.57
1:AAA:267:VAL:HG13	1:AAA:299:LEU:HD23	1.88	0.55
1:BBB:255:CYS:HA	1:BBB:259:LEU:HB2	1.90	0.54
1:BBB:207:TYR:CG	1:BBB:245:GLY:HA3	2.43	0.54
1:BBB:272:TRP:HH2	1:BBB:295:ALA:HB1	1.72	0.53
1:BBB:146:CYS:HA	1:BBB:204:ARG:HD3	1.92	0.52
1:BBB:100:PHE:O	1:BBB:131:ARG:HD3	2.10	0.52
1:BBB:249:LYS:HD2	1:BBB:268:ASP:HB3	1.92	0.51
1:BBB:151:ASN:O	1:BBB:155:ILE:HG13	2.11	0.51
1:AAA:22:LEU:CA	1:AAA:87:ARG:HG2	2.41	0.49
1:AAA:34:ARG:HA	1:AAA:68:GLN:HE22	1.77	0.48
1:AAA:122:ARG:NH2	1:BBB:270:HIS:CE1	2.82	0.48
1:BBB:292:SER:N	1:BBB:293:PRO:CD	2.76	0.48
1:AAA:272:TRP:HH2	1:AAA:295:ALA:HB1	1.80	0.47
1:CCC:139:GLU:HG3	1:CCC:181:PHE:CD1	2.49	0.47
1:CCC:35:LEU:H	1:CCC:68:GLN:HE22	1.62	0.46
1:CCC:79:ARG:NH2	1:CCC:87:ARG:O	2.49	0.46
1:CCC:19:SER:HB3	1:CCC:22:LEU:HB2	1.98	0.45
1:CCC:251:ALA:O	1:CCC:255:CYS:SG	2.74	0.45
1:CCC:164:GLN:HA	1:CCC:179:HIS:CD2	2.52	0.45
1:AAA:164:GLN:HA	1:AAA:179:HIS:CG	2.51	0.45
1:BBB:53:ALA:O	1:BBB:67:THR:OG1	2.30	0.44
1:BBB:163:CYS:O	1:BBB:167:GLY:CA	2.67	0.43
1:AAA:64:TRP:CZ2	1:AAA:96:LEU:HD11	2.53	0.43
1:CCC:233:TYR:HB2	1:CCC:263:GLN:NE2	2.34	0.43
1:CCC:266:PRO:HD2	1:CCC:315:GLN:NE2	2.30	0.43
1:BBB:266:PRO:HD2	1:BBB:315:GLN:NE2	2.30	0.42
1:BBB:132:LEU:HD21	1:BBB:256:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:163:CYS:O	1:BBB:167:GLY:HA3	2.20	0.41
1:CCC:292:SER:HB2	1:CCC:293:PRO:HD2	2.02	0.41
1:AAA:14:ARG:NH1	1:AAA:76:THR:OG1	2.53	0.41
1:BBB:53:ALA:O	1:BBB:67:THR:CB	2.69	0.40
1:BBB:109:LEU:HB3	1:BBB:113:TRP:CH2	2.55	0.40
1:CCC:270:HIS:O	1:CCC:273:GLN:HB3	2.21	0.40
1:BBB:231:ALA:O	1:BBB:261:LYS:NZ	2.52	0.40
1:BBB:79:ARG:NH2	1:BBB:92:GLU:OE1	2.54	0.40

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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	AAA	305/318~(96%)	289~(95%)	15~(5%)	1 (0%)	41 64
1	BBB	306/318~(96%)	288~(94%)	18 (6%)	0	100 100
1	CCC	309/318~(97%)	291 (94%)	17 (6%)	1 (0%)	41 64
All	All	920/954~(96%)	868 (94%)	50 (5%)	2~(0%)	47 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	285	THR
1	AAA	82	ASP

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	AAA	263/266~(99%)	262 (100%)	1 (0%)	91	97
1	BBB	261/266~(98%)	260 (100%)	1 (0%)	91	97
1	CCC	249/266~(94%)	248 (100%)	1 (0%)	91	97
All	All	773/798~(97%)	770 (100%)	3~(0%)	91	97

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	174	ASP
1	BBB	285	THR
1	CCC	82	ASP

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

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

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



Mol	Turne	Chain	Res	Link	Bond lengths			B	ond ang	gles
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SEQ	AAA	401	-	21,23,23	1.07	2 (9%)	30,32,32	2.49	8 (26%)
2	SEQ	CCC	401	-	21,23,23	1.14	2 (9%)	30,32,32	2.90	11 (36%)
2	SEQ	BBB	401	-	21,23,23	1.03	1 (4%)	30,32,32	2.73	9 (30%)

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).

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	SEQ	AAA	401	-	-	0/8/18/18	0/4/4/4
2	SEQ	CCC	401	-	-	0/8/18/18	0/4/4/4
2	SEQ	BBB	401	-	-	1/8/18/18	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	CCC	401	SEQ	C12-C07	2.41	1.47	1.44
2	AAA	401	SEQ	C12-C07	2.14	1.47	1.44
2	BBB	401	SEQ	C12-C07	2.08	1.47	1.44
2	AAA	401	SEQ	C09-C08	2.07	1.41	1.36
2	CCC	401	SEQ	C09-C08	2.07	1.41	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	CCC	401	SEQ	C02-C03-C04	8.93	129.61	119.43
2	BBB	401	SEQ	C01-C03-C04	8.23	128.81	119.43
2	AAA	401	SEQ	C02-C03-C04	7.75	128.27	119.43
2	BBB	401	SEQ	C02-C03-C04	7.69	128.20	119.43
2	CCC	401	SEQ	C01-C03-C04	7.04	127.46	119.43
2	AAA	401	SEQ	C01-C03-C04	6.35	126.67	119.43
2	CCC	401	SEQ	C04-N05-C06	5.24	120.09	116.54
2	BBB	401	SEQ	C04-N05-C06	4.96	119.90	116.54
2	CCC	401	SEQ	C07-C12-N13	4.29	124.67	120.63
2	CCC	401	SEQ	C07-C06-N05	-4.25	118.30	122.81
2	AAA	401	SEQ	C12-C07-C06	4.03	118.41	115.88
2	CCC	401	SEQ	C12-C07-C06	4.01	118.40	115.88

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	AAA	401	SEQ	C07-C12-N13	3.96	124.36	120.63
2	BBB	401	SEQ	C07-C06-N05	-3.85	118.73	122.81
2	AAA	401	SEQ	C07-C06-N05	-3.75	118.83	122.81
2	BBB	401	SEQ	C12-C07-C06	3.75	118.24	115.88
2	BBB	401	SEQ	C07-C12-N13	3.23	123.67	120.63
2	AAA	401	SEQ	C04-N05-C06	3.15	118.68	116.54
2	CCC	401	SEQ	C16-C15-C14	2.69	116.17	111.11
2	CCC	401	SEQ	C12-N13-C14	-2.59	119.24	124.16
2	BBB	401	SEQ	C12-N13-C14	-2.46	119.49	124.16
2	BBB	401	SEQ	C07-C12-N20	-2.33	118.15	121.98
2	CCC	401	SEQ	C07-C12-N20	-2.26	118.28	121.98
2	CCC	401	SEQ	C04-N20-C12	2.24	121.08	117.20
2	BBB	401	SEQ	C04-N20-C12	2.21	121.02	117.20
2	AAA	401	SEQ	C07-C12-N20	-2.14	118.47	121.98
2	AAA	401	SEQ	C12-N13-C14	-2.10	120.17	124.16
2	CCC	401	SEQ	C17-C16-C15	2.04	115.57	111.42

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There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	401	SEQ	C01-C03-C04-N05

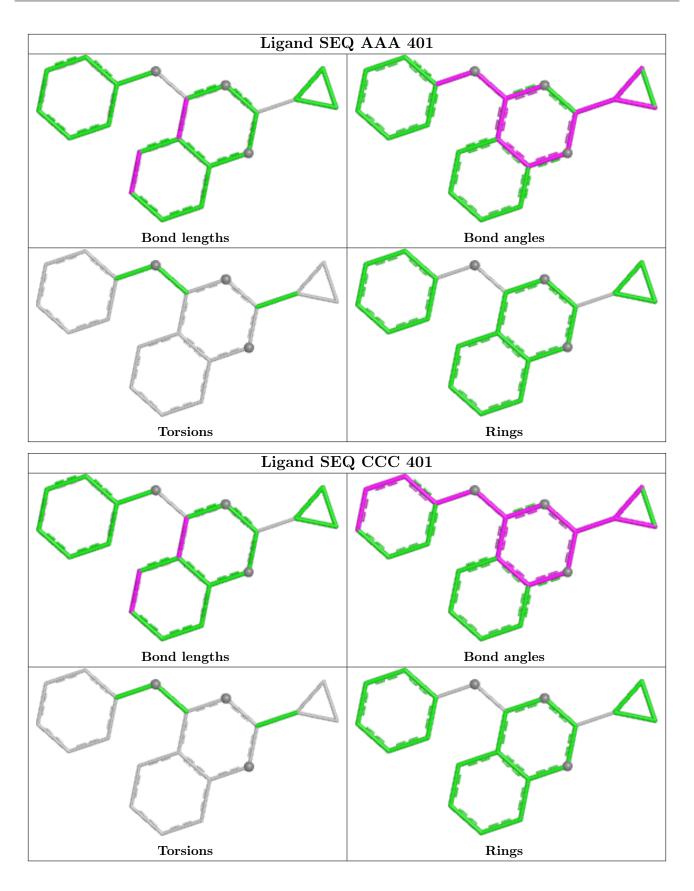
There are no ring outliers.

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.

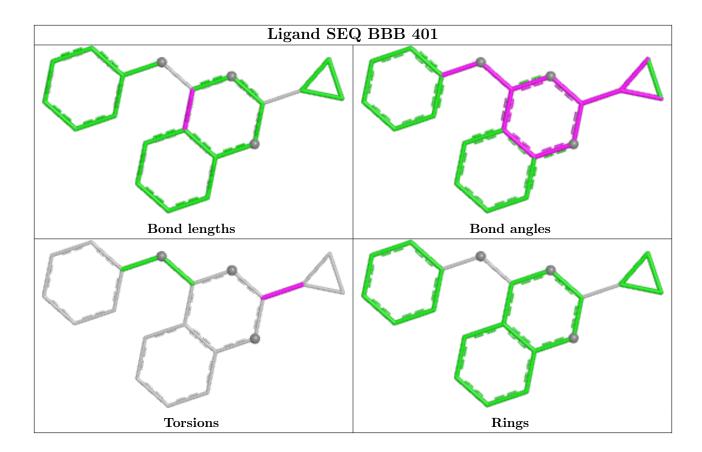












### 5.7 Other polymers (i)

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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	AAA	311/318~(97%)	0.13	3 (0%) 82 80	42, 65, 114, 147	0
1	BBB	310/318~(97%)	0.26	12 (3%) 39 32	46, 73, 112, 140	0
1	CCC	313/318~(98%)	0.31	15 (4%) 30 24	47, 90, 144, 167	0
All	All	934/954~(97%)	0.23	30 (3%) 47 40	42, 76, 134, 167	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	287	GLN	4.3
1	BBB	81	ASP	4.2
1	BBB	286	SER	4.2
1	CCC	234	GLU	3.8
1	CCC	191	GLU	3.4
1	BBB	80	GLY	3.3
1	CCC	80	GLY	3.1
1	BBB	171	ILE	3.0
1	CCC	189	GLY	2.9
1	BBB	84	GLN	2.8
1	CCC	185	HIS	2.8
1	CCC	142	PHE	2.8
1	CCC	149	ASN	2.5
1	BBB	70	GLU	2.5
1	CCC	82	ASP	2.5
1	BBB	10	HIS	2.4
1	AAA	81	ASP	2.4
1	CCC	81	ASP	2.4
1	AAA	78	TYR	2.3
1	BBB	323	LEU	2.3
1	CCC	125	GLN	2.2
1	BBB	175	ASP	2.2
1	BBB	226	GLN	2.2

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Mol	Chain	$\mathbf{Res}$	Type	RSRZ			
1	CCC	216	LEU	2.2			
1	CCC	214	ALA	2.2			
1	AAA	91	GLU	2.2			
1	BBB	126	LYS	2.1			
1	BBB	173	LEU	2.1			
1	CCC	61	ASP	2.1			
1	CCC	97	HIS	2.1			

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### 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.

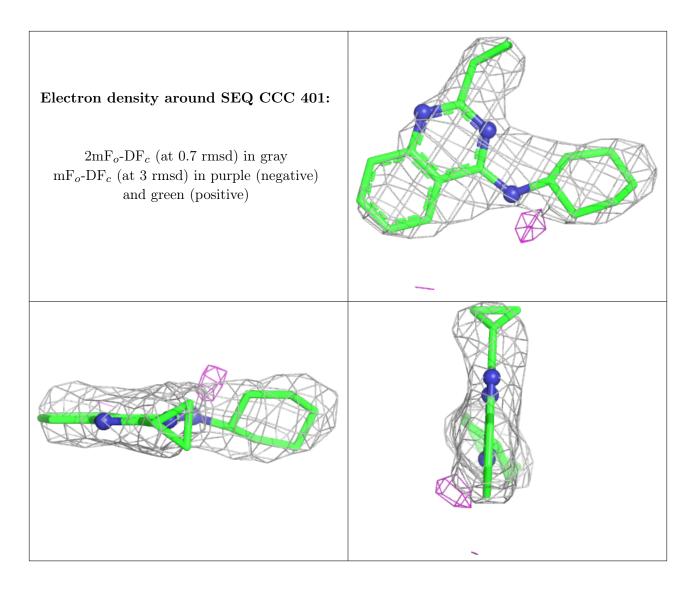
#### 6.4 Ligands (i)

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,  $95^{th}$  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.

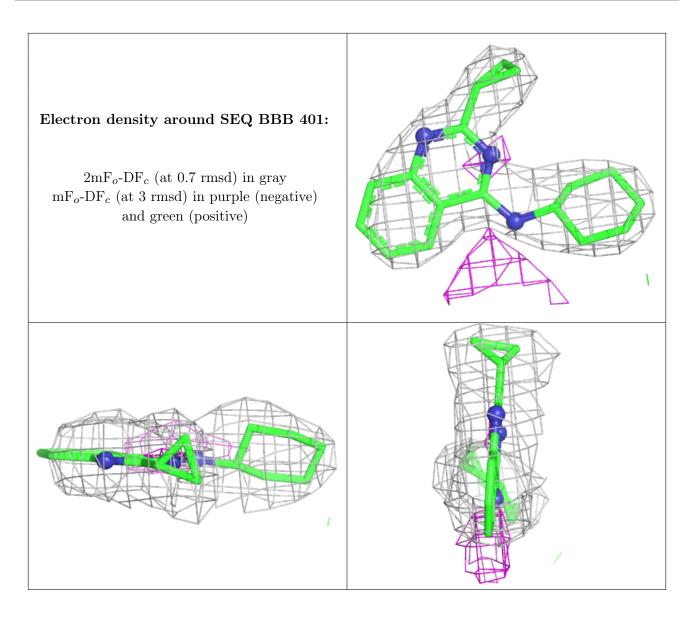
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
2	SEQ	CCC	401	20/20	0.85	0.34	84,97,103,104	0
2	SEQ	BBB	401	20/20	0.86	0.28	57,69,75,78	0
2	SEQ	AAA	401	20/20	0.96	0.19	44,48,55,55	0
3	NI	AAA	402	1/1	0.99	0.19	52,52,52,52	0

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.

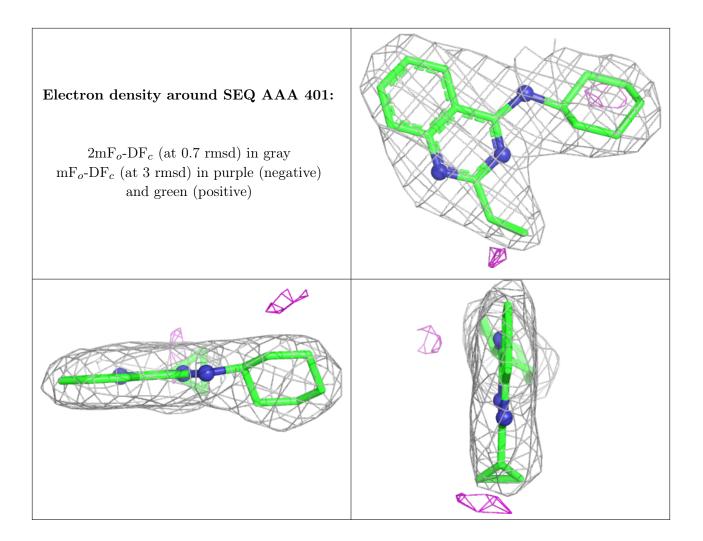












## 6.5 Other polymers (i)

There are no such residues in this entry.

