

Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 04:38 pm GMT

PDB ID : 2XB9

Title: Structure of Helicobacter pylori type II dehydroquinase in complex with in-

hibitor compound (2R)-2-(4-methoxybenzyl)-3-dehydroquinic acid

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Raaij, M.J.

Deposited on : 2010-04-08

Resolution : 2.75 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

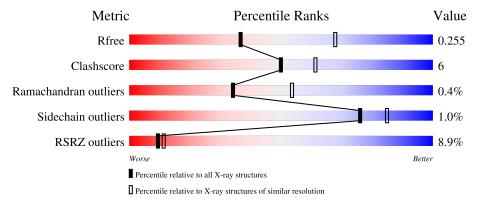
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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		
-		4.0=	9%		
1	A	167	87%	7%	• 5%
_	ъ	105	9%		_
1	В	167	81%	13%	5%
	~		7%		
1	\mathbf{C}	167	85%	10%	5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	С	201	-	X	-	-



2 Entry composition (i)

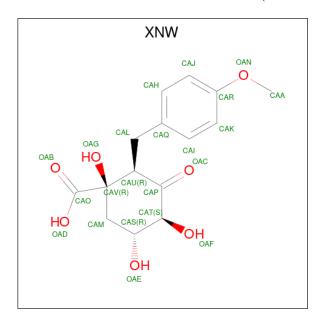
There are 4 unique types of molecules in this entry. The entry contains 3741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	158	Total	С	N	О	S	0	0 0	0
1	A	156	1221	776	205	229	11	0		
1	D	158	Total	С	N	О	S	0	0	0
1	Ъ	198	1221	776	205	229	11	0	0	0
1	С	150	Total	С	N	О	S	0	0	0
	158	1221	776	205	229	11	0		U	

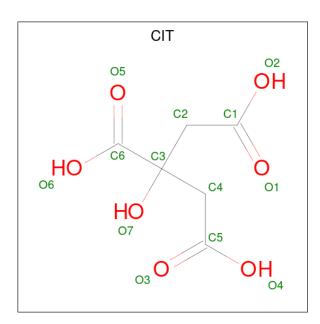
• Molecule 2 is (1R,2R,4S,5R)-1,4,5-TRIHYDROXY-2-(4-METHOXYBENZYL)-3-OXOCYC LOHEXANECARBOXYLIC ACID (three-letter code: XNW) (formula: C₁₅H₁₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 22 15 7	0	0
2	В	1	Total C O	0	0

• Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	С	1	Total 13	C 6	O 7	0	0

• Molecule 4 is water.

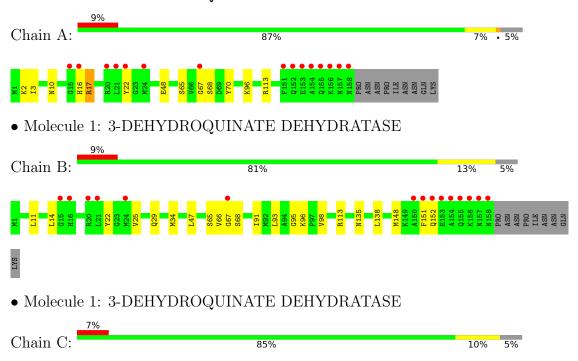
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	В	4	Total O 4 4	0	0
4	С	7	Total O 7 7	0	0



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: 3-DEHYDROQUINATE DEHYDRATASE





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 42 2 2	Depositor	
Cell constants	$100.56\text{\AA} 100.56\text{Å} 105.45\text{Å}$	Donositon	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	34.22 - 2.75	Depositor	
Resolution (A)	34.22 - 2.75	EDS	
% Data completeness	99.8 (34.22-2.75)	Depositor	
(in resolution range)	99.8 (34.22-2.75)	EDS	
R_{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.71 (at 2.76Å)	Xtriage	
Refinement program	REFMAC 5.5.0072	Depositor	
R, R_{free}	0.185 , 0.250	Depositor	
10, 10 free	0.188 , 0.255	DCC	
R_{free} test set	748 reflections (5.13%)	wwPDB-VP	
Wilson B-factor (\mathring{A}^2)	52.2	Xtriage	
Anisotropy	0.189	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.33 \; , 44.2$	EDS	
L-test for twinning ²	$< L > = 0.51, < L^2> = 0.35$	Xtriage	
Estimated twinning fraction	0.127 for -h,l,k	Xtriage	
Estimated twinning fraction	0.035 for -l,-k,-h	Atriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	3741	wwPDB-VP	
Average B, all atoms (Å ²)	45.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: CIT, XNW

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
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.69	0/1241	0.68	0/1672
1	В	0.67	0/1241	0.69	0/1672
1	С	0.63	0/1241	0.67	0/1672
All	All	0.66	0/3723	0.68	0/5016

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1
1	С	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	67	GLY	Peptide
1	С	67	GLY	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	1221	0	1222	13	0
1	В	1221	0	1222	19	0
1	С	1221	0	1222	12	0
2	A	22	0	17	8	0
2	В	22	0	17	6	0
3	С	13	0	5	1	0
4	A	10	0	0	0	0
4	В	4	0	0	0	0
4	С	7	0	0	0	0
All	All	3741	0	3705	43	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 6.

All (43) 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:22:TYR:CE1	2:A:201:XNW:CAH	2.61	0.84
1:A:22:TYR:CE1	2:A:201:XNW:HAH	2.15	0.81
1:A:113:ARG:NH1	2:A:201:XNW:OAF	2.15	0.79
1:B:22:TYR:CE1	2:B:201:XNW:CAH	2.65	0.79
1:B:65:SER:O	1:B:96:LYS:NZ	2.20	0.75
1:B:66:VAL:HG21	1:C:13:MET:CE	2.20	0.71
1:B:22:TYR:CE1	2:B:201:XNW:HAH	2.28	0.69
1:B:91:ILE:HG23	1:B:98:VAL:HG21	1.82	0.61
1:C:16:HIS:O	1:C:16:HIS:CD2	2.54	0.61
2:A:201:XNW:OAC	2:A:201:XNW:HAI	2.00	0.60
1:C:91:ILE:HG23	1:C:98:VAL:HG21	1.83	0.60
1:C:34:MET:HA	1:C:135:ASN:HD21	1.68	0.59
1:B:22:TYR:CD1	2:B:201:XNW:HAH	2.38	0.58
1:A:48:GLU:OE1	1:A:70:TYR:OH	2.21	0.57
1:A:68:SER:HB3	1:A:96:LYS:HZ1	1.72	0.54
1:B:66:VAL:HG21	1:C:13:MET:HE1	1.89	0.53
1:A:68:SER:HB3	1:A:96:LYS:NZ	2.24	0.53
1:B:47:LEU:HD21	1:B:138:LEU:HD21	1.90	0.53
1:C:17:ARG:NH1	3:C:201:CIT:O3	2.39	0.52
1:A:16:HIS:C	1:A:17:ARG:HG2	2.30	0.52
1:C:3:ILE:HD12	1:C:141:MET:HG2	1.90	0.52
1:B:93:LEU:HD22	1:C:17:ARG:HG2	1.90	0.52
1:B:95:GLY:O	1:B:96:LYS:HG3	2.12	0.50

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A + 1	A40 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
1:B:66:VAL:HG21	1:C:13:MET:HE2	1.92	0.49
1:B:22:TYR:CD1	2:B:201:XNW:CAH	2.97	0.47
1:B:34:MET:HA	1:B:135:ASN:HD21	1.80	0.47
1:B:148:MET:HB3	1:B:152:GLN:NE2	2.29	0.47
1:A:22:TYR:CD1	2:A:201:XNW:HAH	2.49	0.47
1:C:33:ILE:HG22	1:C:135:ASN:OD1	2.16	0.46
1:B:68:SER:HB3	1:B:96:LYS:NZ	2.30	0.46
1:B:25:VAL:HG13	1:B:29:GLN:HB2	2.00	0.43
2:A:201:XNW:OAC	2:A:201:XNW:CAI	2.66	0.43
1:A:2:LYS:O	1:A:3:ILE:HD13	2.19	0.43
1:A:16:HIS:C	1:A:17:ARG:CG	2.86	0.43
2:B:201:XNW:OAC	2:B:201:XNW:HAI	2.19	0.43
1:B:11:LEU:O	1:B:14:LEU:HB2	2.19	0.42
1:A:16:HIS:O	1:A:17:ARG:HG2	2.20	0.41
1:C:16:HIS:O	1:C:16:HIS:CG	2.73	0.41
1:C:38:VAL:HA	1:C:43:LEU:HD12	2.01	0.41
1:B:113:ARG:NH1	2:B:201:XNW:OAF	2.54	0.41
1:A:10:ASN:HB3	2:A:201:XNW:HAK	2.03	0.40
1:B:151:PHE:CD1	1:B:151:PHE:C	2.95	0.40
1:A:22:TYR:CZ	2:A:201:XNW:CAH	3.02	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	Perce	ntiles
1	A	156/167 (93%)	149 (96%)	6 (4%)	1 (1%)	25	42
1	В	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
1	С	156/167 (93%)	148 (95%)	7 (4%)	1 (1%)	25	42
All	All	468/501 (93%)	448 (96%)	18 (4%)	2 (0%)	34	53



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLY
1	С	44	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	130/139 (94%)	128 (98%)	2 (2%)	65 78
1	В	130/139 (94%)	130 (100%)	0	100 100
1	С	130/139 (94%)	128 (98%)	2 (2%)	65 78
All	All	390/417 (94%)	386 (99%)	4 (1%)	76 85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	65	SER
1	С	24	MET
1	С	65	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	16	HIS

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)

3 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	Tune	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	Bond lengths		В	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2												
3	CIT	С	201	-	12,12,12	1.18	1 (8%)	17,17,17	2.67	9 (52%)												
2	XNW	A	201	-	21,23,23	1.55	4 (19%)	21,34,34	1.20	3 (14%)												
2	XNW	В	201	-	21,23,23	1.73	2 (9%)	21,34,34	1.75	4 (19%)												

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	CIT	С	201	-	-	9/16/16/16	-
2	XNW	A	201	-	-	1/12/35/35	0/2/2/2
2	XNW	В	201	_	-	3/12/35/35	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\text{\AA})$
2	В	201	XNW	CAS-CAT	4.26	1.57	1.52
2	В	201	XNW	CAL-CAQ	3.57	1.59	1.51
2	A	201	XNW	CAS-CAT	3.07	1.55	1.52
2	A	201	XNW	CAT-CAP	3.01	1.55	1.52
2	A	201	XNW	CAL-CAU	-2.72	1.50	1.54
2	A	201	XNW	CAL-CAQ	2.69	1.57	1.51
3	С	201	CIT	C3-C6	-2.69	1.50	1.53



All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	201	XNW	CAQ-CAL-CAU	5.27	123.08	113.42
3	С	201	CIT	O6-C6-C3	4.81	121.40	113.05
3	С	201	CIT	C4-C3-C6	-4.22	101.03	110.11
3	С	201	CIT	O2-C1-C2	4.11	127.56	114.35
3	С	201	CIT	O2-C1-O1	-3.85	113.70	123.30
3	С	201	CIT	O4-C5-C4	2.91	123.70	114.35
2	A	201	XNW	CAQ-CAL-CAU	2.63	118.24	113.42
2	В	201	XNW	CAL-CAQ-CAI	2.61	126.09	120.91
2	В	201	XNW	CAJ-CAR-CAK	-2.47	116.37	120.18
3	С	201	CIT	O5-C6-C3	-2.39	118.88	122.25
2	В	201	XNW	CAI-CAK-CAR	2.28	122.53	119.73
3	С	201	CIT	C4-C3-C2	2.27	115.07	109.16
3	С	201	CIT	O7-C3-C6	-2.24	105.72	108.86
3	С	201	CIT	O7-C3-C4	2.11	114.33	109.40
2	A	201	XNW	OAF-CAT-CAS	2.08	113.82	110.28
2	A	201	XNW	CAJ-CAR-CAK	-2.04	117.03	120.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	201	CIT	C1-C2-C3-C4
3	С	201	CIT	C1-C2-C3-C6
3	С	201	CIT	C2-C3-C4-C5
3	С	201	CIT	O7-C3-C4-C5
3	С	201	CIT	C6-C3-C4-C5
3	С	201	CIT	C1-C2-C3-O7
2	В	201	XNW	CAK-CAR-OAN-CAA
2	В	201	XNW	CAJ-CAR-OAN-CAA
3	С	201	CIT	C2-C3-C6-O5
3	С	201	CIT	O2-C1-C2-C3
3	С	201	CIT	O1-C1-C2-C3
2	A	201	XNW	OAD-CAO-CAV-OAG
2	В	201	XNW	OAD-CAO-CAV-OAG

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	201	CIT	1	0

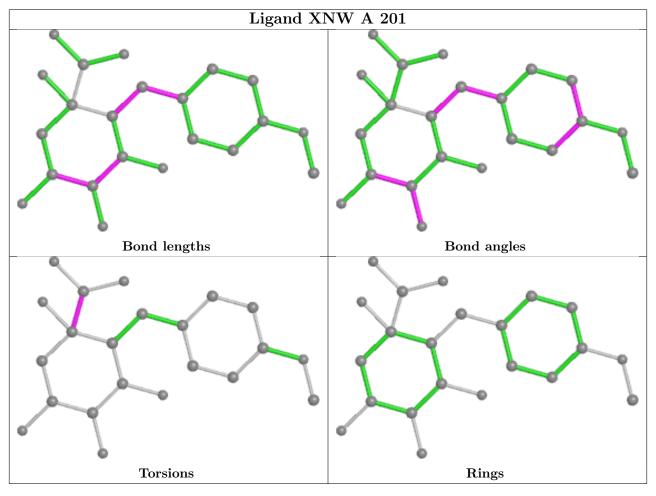
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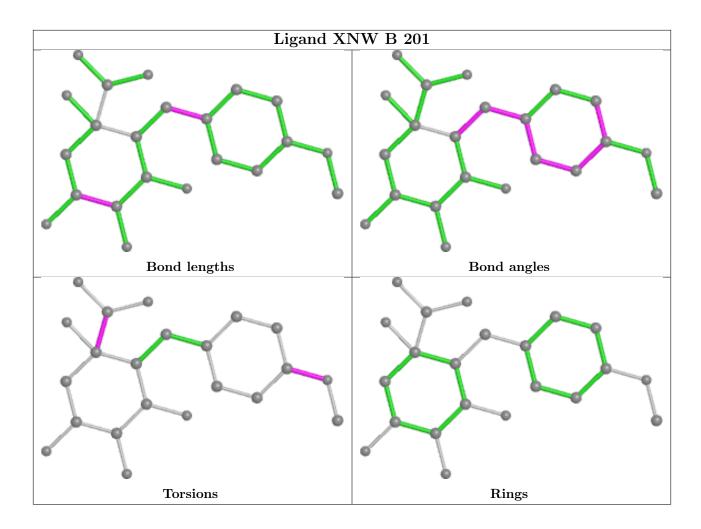
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	XNW	8	0
2	В	201	XNW	6	0

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 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	<RSRZ $>$ #RSRZ $>$ 2		$OWAB(\AA^2)$	Q<0.9
1	A	158/167 (94%)	0.17	15 (9%) 8 9	21, 36, 85, 104	0
1	В	158/167 (94%)	0.22	15 (9%) 8 9	24, 40, 87, 106	0
1	С	158/167 (94%)	0.31	12 (7%) 13 16	21, 41, 95, 114	0
All	All	474/501 (94%)	0.24	42 (8%) 9 11	21, 39, 93, 114	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	155	GLN	10.1
1	A	157	ASN	8.3
1	С	156	LYS	8.1
1	С	157	ASN	7.7
1	С	155	GLN	7.7
1	В	154	ALA	7.5
1	В	157	ASN	7.5
1	A	158	ASN	7.0
1	С	158	ASN	7.0
1	В	158	ASN	6.7
1	С	154	ALA	6.5
1	A	155	GLN	6.3
1	С	152	GLN	6.3
1	В	152	GLN	5.2
1	В	151	PHE	5.1
1	A	156	LYS	4.6
1	В	156	LYS	4.6
1	С	151	PHE	4.4
1	A	152	GLN	4.4
1	A	151	PHE	4.3
1	В	153	GLU	4.1
1	A	154	ALA	3.6
1	В	15	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	С	153	GLU	3.5
1	С	24	MET	3.4
1	В	16	HIS	3.2
1	A	67	GLY	3.0
1	A	15	GLY	3.0
1	В	20	ARG	2.8
1	A	153	GLU	2.7
1	В	150	ALA	2.6
1	С	20	ARG	2.6
1	A	21	LEU	2.5
1	A	24	MET	2.4
1	С	22	TYR	2.3
1	A	20	ARG	2.3
1	В	24	MET	2.3
1	A	16	HIS	2.1
1	С	40	GLN	2.1
1	В	21	LEU	2.1
1	В	67	GLY	2.1
1	A	22	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

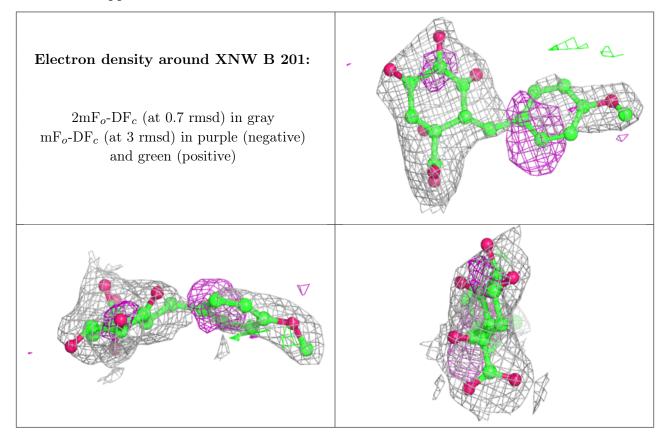
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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.

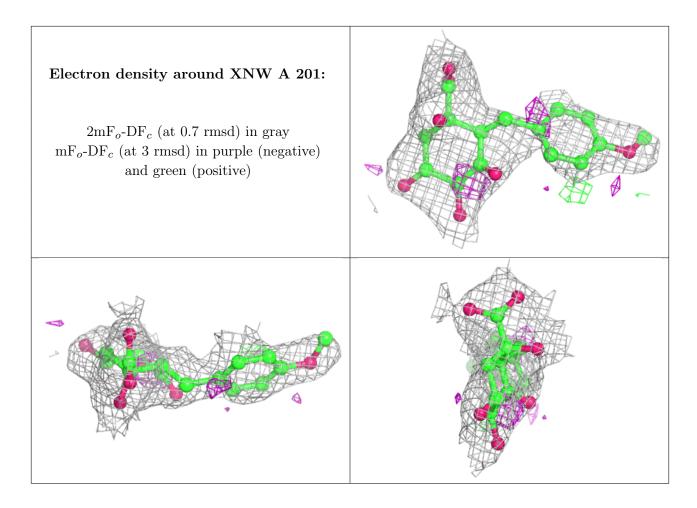
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	XNW	В	201	22/22	0.90	0.26	30,40,50,51	0
2	XNW	A	201	22/22	0.92	0.23	28,38,47,47	0
3	CIT	С	201	13/13	0.93	0.20	38,40,45,46	0



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.

