

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

#### Sep 24, 2024 - 04:17 pm BST

PDB ID	:	8R1M
Title	:	Structure of TxGH116 with covalently bound N-azido-octyl aziridine
Authors	:	Offen, W.A.; Davies, G.J.
Deposited on		
Resolution	:	1.90  Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

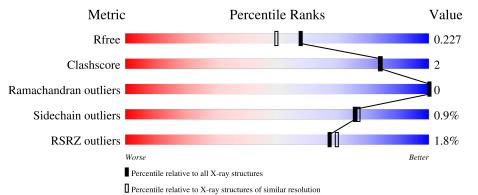
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 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 1.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	А	799	90%	6%	•
1	В	799	<sup>2%</sup> 92%	5%	·



#### 8 R1 M

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25664 atoms, of which 12139 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	772	Total 12413	C 4082	H 6089	N 1015	O 1199	S 28	187	25	0
1	В	772	Total 12270	C 4048	Н 6002	N 1002	0 1191	S 27	198	16	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	16	ALA	-	expression tag	UNP F6BL85
А	17	MET	-	expression tag	UNP F6BL85
А	18	ALA	-	expression tag	UNP F6BL85
А	807	LEU	-	expression tag	UNP F6BL85
А	808	GLU	-	expression tag	UNP F6BL85
А	809	HIS	-	expression tag	UNP F6BL85
А	810	HIS	-	expression tag	UNP F6BL85
А	811	HIS	-	expression tag	UNP F6BL85
А	812	HIS	-	expression tag	UNP F6BL85
А	813	HIS	-	expression tag	UNP F6BL85
А	814	HIS	-	expression tag	UNP F6BL85
В	16	ALA	-	expression tag	UNP F6BL85
В	17	MET	-	expression tag	UNP F6BL85
В	18	ALA	-	expression tag	UNP F6BL85
В	807	LEU	-	expression tag	UNP F6BL85
В	808	GLU	-	expression tag	UNP F6BL85
В	809	HIS	-	expression tag	UNP F6BL85
В	810	HIS	-	expression tag	UNP F6BL85
В	811	HIS	-	expression tag	UNP F6BL85
В	812	HIS	-	expression tag	UNP F6BL85
В	813	HIS	-	expression tag	UNP F6BL85
В	814	HIS	_	expression tag	UNP F6BL85

There are 22 discrepancies between the modelled and reference sequences:

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

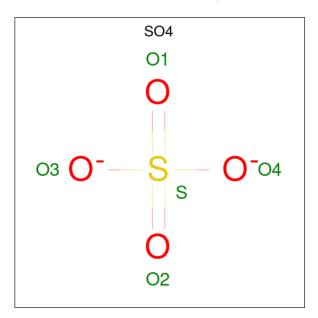


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Cl 2 2	0	0
3	В	1	Total Cl 1 1	0	0

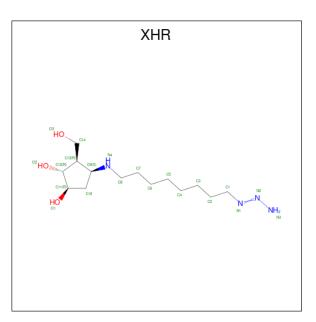
• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is (1R,2R,3R,4S)-4-[8-(azanyldiazenyl)octylamino]-3-(hydroxymethyl)cyclopenta ne-1,2-diol (three-letter code: XHR) (formula: C<sub>14</sub>H<sub>30</sub>N<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
5	5 A	1	Total	С	Η	Ν	Ο	6	0	
0		1	42	13	25	1	3	0	0	
Б	r D	D 1	Total	С	Η	Ν	Ο	6	0	
5	D	1	39	12	23	1	3	0		

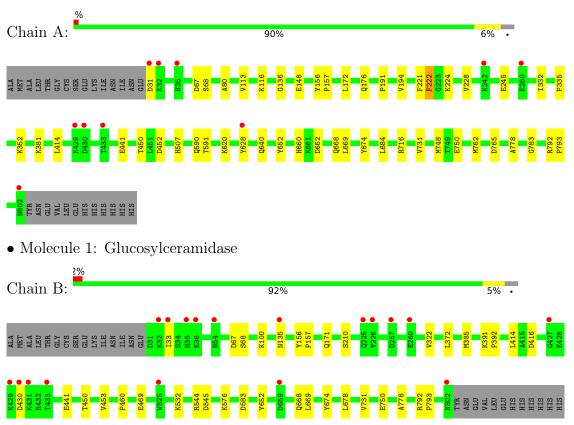
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	455	Total O 455 455	0	0
6	В	425	Total         O           425         425	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: Glucosylceramidase



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	54.98Å 165.15Å 178.92Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	56.09 - 1.90	Depositor
	56.09 - 1.90	EDS
% Data completeness	99.9 (56.09-1.90)	Depositor
(in resolution range)	99.9(56.09-1.90)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.56 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
D D.	0.177 , $0.227$	Depositor
$R, R_{free}$	0.177 , $0.227$	DCC
$R_{free}$ test set	6306 reflections $(4.88%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.7	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36, $39.3$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25664	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 31.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1884e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: SO4, XHR, CA, CL

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	А	0.40	0/6595	0.77	1/8942~(0.0%)	
1	В	0.41	0/6506	0.77	0/8827	
All	All	0.41	0/13101	0.77	1/17769~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	748	MET	CG-SD-CE	5.20	108.51	100.20

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	А	6324	6089	5983	32	0
1	В	6268	6002	5910	23	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	2	0	0	0	0
3	В	1	0	0	0	0
4	А	10	0	0	0	0
4	В	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	$H(model) \mid H(added) \mid$		Symm-Clashes
5	А	17	25	0	0	0
5	В	16	23	0	0	0
6	А	455	0	0	11	0
6	В	425	0	0	5	0
All	All	13525	12139	11893	55	0

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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 2.

The worst 5 of 55 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:352:LYS:CE	6:A:1001:HOH:O	1.98	1.12	
1:B:576:LYS:HG3	1:B:583:ASP:OD2	1.81	0.80	
1:B:135:ASN:OD1	6:B:1001:HOH:O	2.03	0.75	
1:A:441:GLU:OE2	1:A:450[B]:THR:HG21	1.93	0.68	
1:A:750:GLU:OE2	6:A:1002:HOH:O	2.13	0.67	

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	Percen	ntiles
1	А	795/799~(100%)	763~(96%)	32~(4%)	0	100	100
1	В	786/799~(98%)	755~(96%)	31 (4%)	0	100	100
All	All	1581/1598~(99%)	1518 (96%)	63~(4%)	0	100	100

There are no Ramachandran outliers to report.



#### 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	Rotameric Outliers	
1	А	669/685~(98%)	663~(99%)	6 (1%)	75 77
1	В	656/685~(96%)	651 (99%)	5 (1%)	79 80
All	All	1325/1370~(97%)	1314 (99%)	11 (1%)	75 80

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	372	LEU
1	В	416	ASP
1	В	674	TYR
1	В	430	ASP
1	А	640	GLN

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

Mol	Chain	Res	Type
1	А	639	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)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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).

Mal	Mol Type Chai		hain Res	Res Link	Bo	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
5	XHR	А	906	1	$17,\!17,\!21$	0.62	0	$14,\!21,\!25$	0.94	1 (7%)	
4	SO4	А	905	-	4,4,4	0.31	0	6,6,6	0.13	0	
5	XHR	В	903	1	16,16,21	0.36	0	13,20,25	0.70	0	
4	SO4	В	904	-	4,4,4	0.35	0	6,6,6	0.08	0	
4	SO4	А	904	-	4,4,4	0.39	0	$6,\!6,\!6$	0.10	0	

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.

I	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	5	XHR	В	903	1	-	1/9/25/30	0/1/1/1
	5	XHR	А	906	1	-	2/10/26/30	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	А	906	XHR	O1-C11-C10	2.62	120.27	110.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

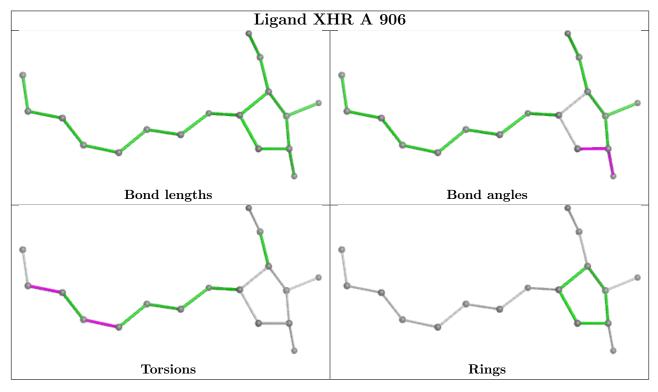
Mol	Chain	Res	Type	Atoms
5	А	906	XHR	C2-C3-C4-C5
5	В	903	XHR	C4-C5-C6-C7
5	А	906	XHR	C4-C5-C6-C7

There are no ring outliers.

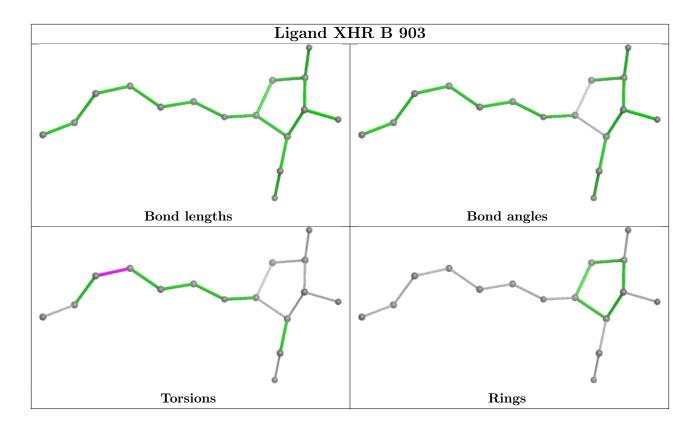


No monomer is involved in short contacts.

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 sufficient 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	$\mathbf{OWAB}(\mathbf{A}^2)$	$Q{<}0.9$
1	А	772/799~(96%)	-0.46	10 (1%) 74 76	9, 22, 39, 57	67~(8%)
1	В	772/799~(96%)	-0.45	18 (2%) 61 63	8, 22, 39, 68	66 (8%)
All	All	1544/1598~(96%)	-0.46	28 (1%) 67 70	8, 22, 39, 68	133 (8%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	429	LYS	7.3
1	В	429	LYS	6.2
1	А	802	ASN	5.2
1	В	430	ASP	4.8
1	А	35	HIS	4.4

## 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.

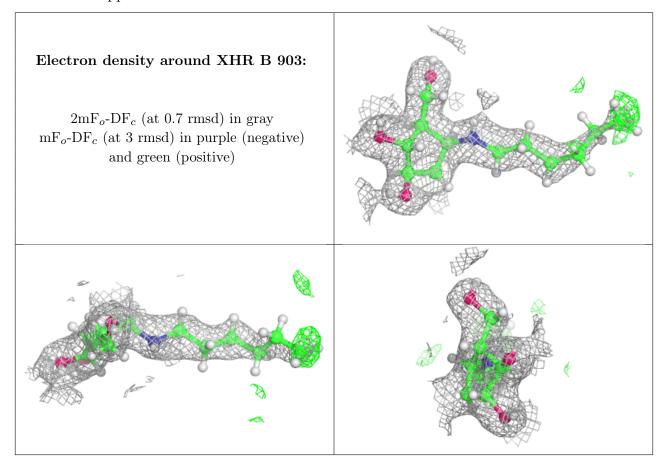
## 6.4 Ligands (i)

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.

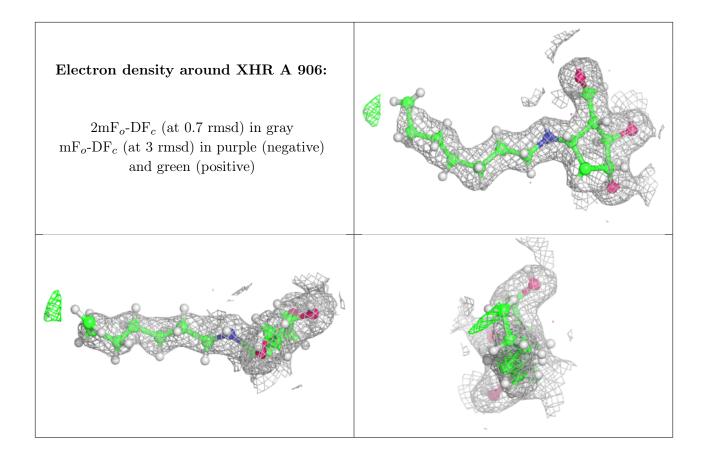


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
4	SO4	А	905	5/5	0.77	0.14	$46,\!52,\!55,\!61$	5
4	SO4	А	904	5/5	0.78	0.20	42,42,44,45	5
4	SO4	В	904	5/5	0.81	0.15	36,37,41,41	5
3	CL	А	902	1/1	0.86	0.13	49,49,49,49	0
3	CL	В	902	1/1	0.91	0.11	$68,\!68,\!68,\!68$	0
5	XHR	В	903	16/21	0.93	0.10	18,24,29,29	13
5	XHR	А	906	17/21	0.94	0.09	18,23,32,33	10
2	CA	В	901	1/1	0.98	0.03	31,31,31,31	0
2	CA	А	901	1/1	0.98	0.03	29,29,29,29	0
3	CL	А	903	1/1	0.99	0.06	19,19,19,19	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.

