

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

#### Aug 29, 2023 – 08:27 PM EDT

PDB ID	:	3MS4
Title	:	Glycogen phosphorylase complexed with 4-trifluoromethylbenzaldehyde-4-(be
		ta-D-glucopyranosyl)-thiosemicarbazone
Authors	:	Alexacou, KM.
Deposited on	:	2010-04-29
Resolution	:	2.07  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 (1)) were used in the production of this report:

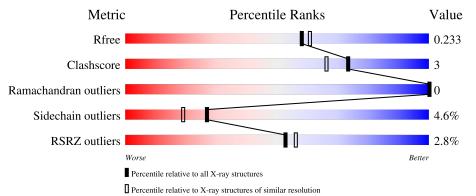
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 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 2.07 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	842	86%	9% • •



#### 3MS4

# 2 Entry composition (i)

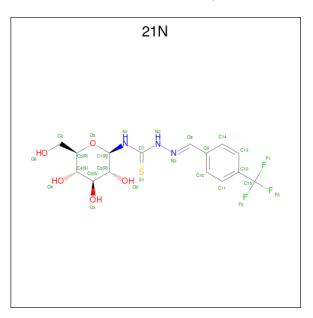
There are 3 unique types of molecules in this entry. The entry contains 6857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	А	810	Total 6610	C 4213	N 1163	O 1204	Р 1	S 29	0	1	0

• Molecule 2 is N-{[(2E)-2-{[4-(trifluoromethyl)phenyl]methylidene}hydrazino]carbonothioyl} -beta-D-glucopyranosylamine (three-letter code: 21N) (formula:  $C_{15}H_{18}F_3N_3O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	Λ	1	Total	С	F	Ν	0	S	0	0
	A	1	27	15	3	3	5	1	0	0
0	٨	1	Total	С	F	Ν	Ο	S	0	0
	A	1	27	15	3	3	5	1	0	U

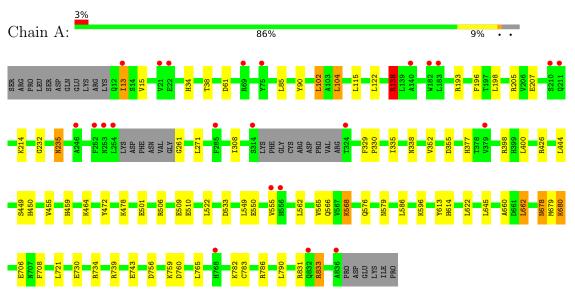
• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	А	193	Total C 193 19	3	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: Glycogen phosphorylase, muscle form



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	128.91Å 128.91Å 116.97Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.43 - 2.07	Depositor
Resolution (A)	51.71 - 2.07	EDS
% Data completeness	93.2 (56.43-2.07)	Depositor
(in resolution range)	93.2(51.71-2.07)	EDS
R <sub>merge</sub>	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.58 (at 2.07 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.2.0019$ , CNS	Depositor
D D.	0.193 , $0.235$	Depositor
$R, R_{free}$	0.191 , $0.233$	DCC
$R_{free}$ test set	2860  reflections  (5.07%)	wwPDB-VP
Wilson B-factor $(Å^2)$	37.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.30,47.3	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6857	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.99% 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: LLP,  $21\mathrm{N}$ 

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).

	Mal	Chain	Bond	lengths	Bond angles		
	Mol	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
ſ	1	А	0.51	0/6737	0.61	2/9117~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	138	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	А	138	ARG	NE-CZ-NH1	-6.46	117.07	120.30

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	6610	0	6542	44	0
2	А	54	0	36	0	0
3	А	193	0	0	4	0
All	All	6857	0	6578	44	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 (44) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:568:LYS:HE2	3:A:895:HOH:O	1.86	0.74
1:A:455:VAL:H	1:A:459:HIS:HD2	1.38	0.71
1:A:138:ARG:O	1:A:138:ARG:HD3	1.94	0.67
1:A:235:ASN:H	1:A:235:ASN:HD22	1.43	0.66
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.79	0.65
1:A:355:ASP:OD1	1:A:398:ARG:HD3	1.96	0.64
1:A:783:CYS:SG	1:A:786:ARG:NH2	2.71	0.64
1:A:261:GLY:N	3:A:1000:HOH:O	2.31	0.63
1:A:678:ASN:HD22	1:A:679:MET:H	1.46	0.62
1:A:449:SER:O	1:A:478:LYS:HE2	2.01	0.61
1:A:13:ILE:HD12	1:A:501:GLU:HB2	1.85	0.58
1:A:565:VAL:HG11	1:A:660:ALA:HB2	1.85	0.58
1:A:730:GLU:O	1:A:734:ARG:HG3	2.06	0.56
1:A:450:HIS:HE1	3:A:933:HOH:O	1.89	0.56
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.89	0.55
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.89	0.54
1:A:549:LEU:HB3	1:A:555:VAL:HG23	1.89	0.53
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.42	0.53
1:A:235:ASN:H	1:A:235:ASN:ND2	2.07	0.51
1:A:15:VAL:HG12	1:A:509:GLU:HG2	1.93	0.51
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.93	0.49
1:A:680:LLP:O3	1:A:680:LLP:NZ	2.44	0.49
1:A:565:VAL:HG11	1:A:660:ALA:CB	2.44	0.48
1:A:614:HIS:HE1	1:A:760:ASP:OD2	1.96	0.48
1:A:550:GLU:HG2	1:A:555:VAL:O	2.13	0.47
1:A:678:ASN:ND2	1:A:679:MET:H	2.12	0.46
1:A:506:ARG:NH1	1:A:533:ASP:OD2	2.48	0.46
1:A:450:HIS:HD2	3:A:934:HOH:O	1.98	0.46
1:A:678:ASN:HD22	1:A:678:ASN:N	2.13	0.46
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.99	0.44
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.83	0.43
1:A:214:LYS:HE2	1:A:214:LYS:HB3	1.81	0.43
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.99	0.43
1:A:308:ILE:HD13	1:A:352:VAL:HG11	2.00	0.43
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.99	0.43
1:A:235:ASN:HD22	1:A:235:ASN:N	2.05	0.42
1:A:464:LYS:HD2	1:A:472:TYR:CE1	2.55	0.41
1:A:756:ASP:O	1:A:759:LYS:HG2	2.20	0.41
1:A:678:ASN:HD22	1:A:679:MET:N	2.15	0.41
1:A:85:LEU:HD12	1:A:85:LEU:N	2.36	0.41
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.85	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ARG:O	1:A:743:GLU:HG3	2.20	0.41
1:A:205:ARG:NH2	1:A:207:GLU:HG3	2.36	0.40
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.86	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	А	804/842~(96%)	776~(96%)	28~(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	Outliers	Percentiles		
1	А	701/730~(96%)	669~(95%)	32~(5%)	27 19		

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	13	ILE
1	А	90	TYR
1	А	102	LEU



Mol	Chain	Res	Type
1	А	104	LEU
1	A A	115	LEU
1		122	LEU
1	А	138	ARG
1	А	198	LEU
1	А	235	ASN
1	А	271	LEU
1	А	400	LEU
1	А	426	ARG
1	А	444	LEU
1	A A	510	GLU
1	А	522	LEU
1	A A	568	LYS
1	А	579	ASN
1	А	586	LEU
1	А	596	LYS
1	A	613	TYR
1	А	622	LEU
1	А	645	LEU
1	А	662	LEU
1	А	678	ASN
1	A A	706	GLU
1	А	708	PHE
1	А	721	LEU
1	А	765	LEU
1	А	782	LYS
1	А	790	LEU
1	А	831	ARG
1	А	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	34	HIS
1	А	73	HIS
1	А	235	ASN
1	А	270	ASN
1	А	325	ASN
1	А	412	ASN
1	А	450	HIS
1	А	459	HIS
1	А	481	ASN



Mol	Chain	Res	Type
1	А	484	ASN
1	А	566	GLN
1	А	579	ASN
1	А	614	HIS
1	А	678	ASN
1	А	727	ASN
1	А	767	HIS
1	А	832	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)

1 non-standard protein/DNA/RNA residue 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).

Ν	പ	Type	Chain	Dog	Link	Bo	ond leng	$\operatorname{ths}$	B	ond ang	les
10.	101	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	1	LLP	А	680	1	23,24,25	1.66	5 (21%)	25,32,34	1.20	4 (16%)

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.

Mo	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	680	1	-	1/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	680	LLP	O3-C3	-5.26	1.24	1.37



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	680	LLP	C4-C4'	2.81	1.52	1.46
1	А	680	LLP	P-OP2	-2.46	1.45	1.54
1	А	680	LLP	C4'-NZ	2.33	1.35	1.27
1	А	680	LLP	C2-N1	2.00	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	680	LLP	CE-NZ-C4'	-2.97	109.78	118.90
1	А	680	LLP	C4-C4'-NZ	-2.28	113.83	124.31
1	А	680	LLP	OP3-P-OP2	2.22	116.13	107.64
1	А	680	LLP	C5-C6-N1	-2.11	120.31	123.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

$\mathbb{N}$	ſol	Chain	Res	Type	Atoms
	1	А	680	LLP	C4-C5-C5'-OP4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	680	LLP	1	0

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

2 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	Type	Chain	Res	es Link	Bo	Bond lengths			Bond angles		
INIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	21N	А	998	-	28,28,28	1.37	2 (7%)	40,40,40	1.03	3 (7%)	
2	21N	А	920	-	28,28,28	1.49	4 (14%)	40,40,40	1.13	3 (7%)	

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	21N	А	998	-	-	1/18/38/38	0/2/2/2
2	21N	А	920	-	-	0/18/38/38	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	998	21N	N2-N3	-5.21	1.31	1.38
2	А	920	21N	N2-N3	-4.62	1.32	1.38
2	А	920	21N	C7-S1	-4.20	1.57	1.68
2	А	998	21N	C7-S1	-3.26	1.60	1.68
2	А	920	21N	C8-N3	-2.60	1.25	1.28
2	А	920	21N	C1-N1	2.15	1.45	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	920	21N	C5-O5-C1	3.43	117.17	112.52
2	А	920	21N	C8-N3-N2	2.63	120.59	115.96
2	А	998	21N	C8-N3-N2	2.49	120.34	115.96
2	А	998	21N	C7-N2-N3	2.42	123.11	120.27
2	А	920	21N	N2-C7-N1	2.05	118.72	115.98
2	А	998	21N	S1-C7-N2	2.02	123.59	119.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

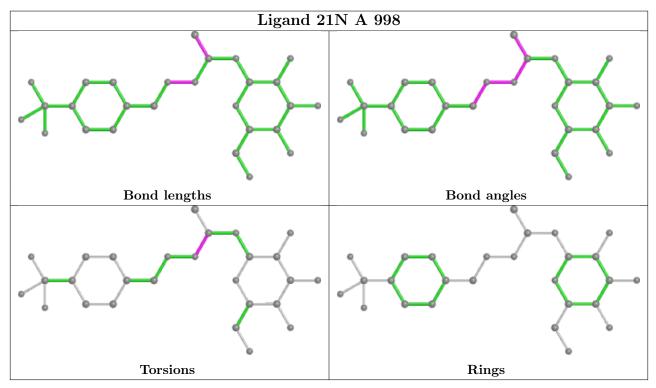
Mol	Chain	Res	Type	Atoms
2	А	998	21N	N1-C7-N2-N3

There are no ring outliers.

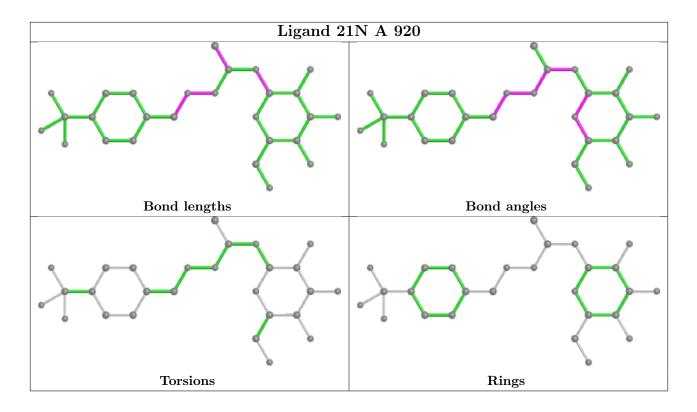
No monomer is involved in short contacts.



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	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	809/842~(96%)	-0.05	23 (2%) 53	56	27, 42, 63, 83	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	252	PHE	5.6
1	А	253	ASN	5.2
1	А	21	VAL	4.7
1	А	324	THR	4.4
1	А	211	GLN	3.6
1	А	836	ALA	3.6
1	А	13	ILE	3.2
1	А	75	TYR	3.1
1	А	556	HIS	2.7
1	А	210	SER	2.7
1	А	22	GLU	2.6
1	А	314	SER	2.5
1	А	183	LEU	2.5
1	А	555	VAL	2.5
1	А	285	PHE	2.5
1	А	832	GLN	2.4
1	А	182	TRP	2.4
1	А	69	ARG	2.3
1	А	768	HIS	2.2
1	А	246	ALA	2.2
1	А	140	ALA	2.1
1	А	254	LEU	2.0
1	А	379	VAL	2.0



#### 6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	LLP	А	680	24/25	0.97	0.14	31,33,36,40	0

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

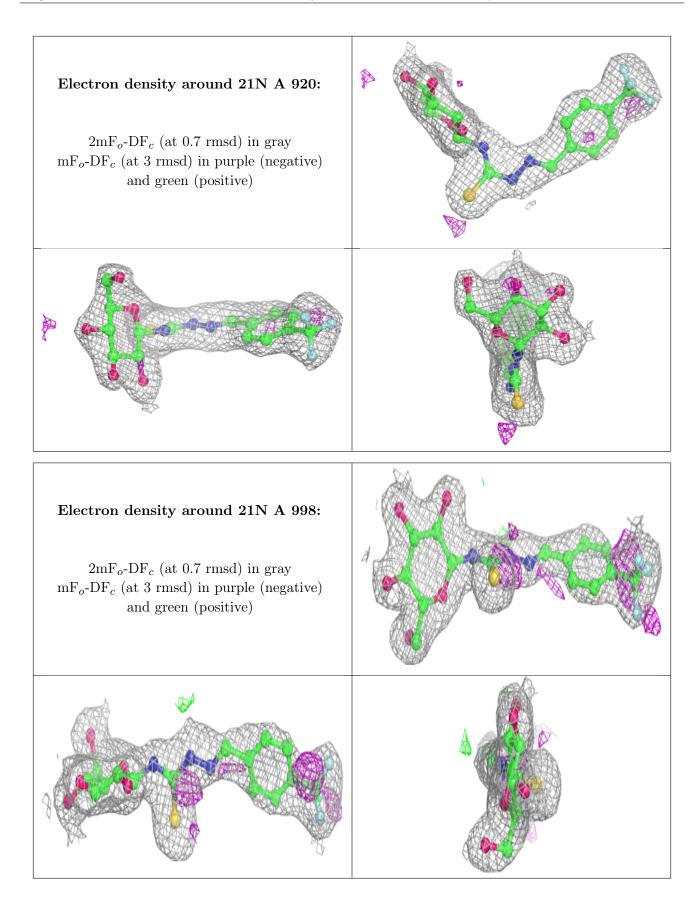
#### 6.4 Ligands (i)

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	21N	А	920	27/27	0.91	0.12	44,47,53,54	0
2	21N	А	998	27/27	0.92	0.12	30,43,54,55	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.

