

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

Jan 30, 2024 – 06:10 PM EST

PDB ID : 8TTY

Title : Crystal structure of monkey TLR7 ectodomain with compound 5

Authors : Critton, D.A. Deposited on : 2023-08-15

Resolution : 2.10 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

Mogul : 1.8.5 (274361), 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)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

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

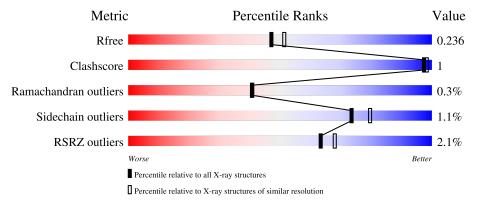
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.10 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 o	f chain
1	A	817	91%	• 6%
1	В	817	90%	• 6%
2	С	3	67%	33%
3	D	2	50%	50%
3	Е	2	50%	50%



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Mol	Chain	Length	Quality	of chain
3	F	2	50%	50%



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25867 atoms, of which 12443 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 Toll-like receptor 7.

Mol	Chain	Residues		Atoms						AltConf	Trace
1	A	768	Total 12216	C 3945	H 6068	N 1031	O 1142	S 30	6068	1	0
1	В	768	Total 12150	C 3936	H 6022	N 1020	O 1142	S 30	6022	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP G8E2R2
A	24	SER	-	expression tag	UNP G8E2R2
A	25	PRO	-	expression tag	UNP G8E2R2
A	26	TRP	-	expression tag	UNP G8E2R2
A	167	GLN	ASN	conflict	UNP G8E2R2
A	389	GLN	ASN	conflict	UNP G8E2R2
A	488	GLN	ASN	conflict	UNP G8E2R2
A	799	GLN	ASN	conflict	UNP G8E2R2
В	23	ARG	-	expression tag	UNP G8E2R2
В	24	SER	-	expression tag	UNP G8E2R2
В	25	PRO	-	expression tag	UNP G8E2R2
В	26	TRP	-	expression tag	UNP G8E2R2
В	167	GLN	ASN	conflict	UNP G8E2R2
В	389	GLN	ASN	conflict	UNP G8E2R2
В	488	GLN	ASN	conflict	UNP G8E2R2
В	799	GLN	ASN	conflict	UNP G8E2R2

• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





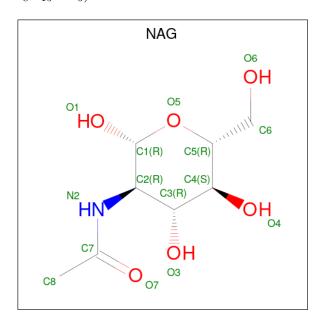
Mol	Chain	Residues		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
2	С	3	Total 73	C 22	H 34	N 2	O 15	34	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
3	D	2	Total	С	Η	N	О	25	0	0	
J 3	D	2	53	16	25	2	10	20	U		
3	Е	2	Total	С	Н	N	О	25	0	0	
9	l Li	2	53	16	25	2	10	20	0	U	
3	E	9	Total	С	Н	N	О	25	0	0	
3	I,	2	53	16	25	2	10	20	U		

 $\bullet$  Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\rm C_8H_{15}NO_6).$ 



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
1	Λ	1	Total	С	Н	N	О	12	0	
4	A	1	27	8	13	1	5	19	U	
1	Λ	1	Total	С	Н	N	О	13	0	
4	A	1	27	8	13	1	5	10	U	

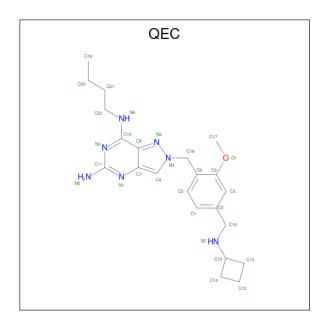


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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
4	A	1	Total	С	Н	N	О	13	0
4	A	1	27	8	13	1	5	13	U
4	A	1	Total	С	Н	N	О	13	0
4	A	1	27	8	13	1	5	13	U
4	A	1	Total	С	Η	N	О	13	0
4	Λ	1	27	8	13	1	5	10	U
4	A	1	Total	С	Н	N	Ο	13	0
-1	11	1	27	8	13	1	5	10	U
4	A	1	Total	С	Η	N	Ο	13	0
<b>T</b>	71	1	27	8	13	1	5	10	Ü
4	В	1	Total	С	Η	N	Ο	13	0
1	Б	1	27	8	13	1	5	10	Ü
4	В	1	Total	С	Η	N	Ο	13	0
		1	27	8	13	1	5	10	Ü
4	В	1	Total	С	Η	N	Ο	13	0
		-	27	8	13	1	5	10	Ŭ
4	В	1	Total	С	Η	N	O	13	0
_	_	_	27	8	13	1	5		Ü
4	В	1	Total	С	Н	N	O	13	0
		-	27	8	13	1	5		Ü
4	В	1	Total	C	H	N	O	13	0
_	_	_	27	8	13	1	5		
4	В	1	Total	$\mathbf{C}$	H	N	O	13	0
		_	27	8	13	1	5		Ŭ

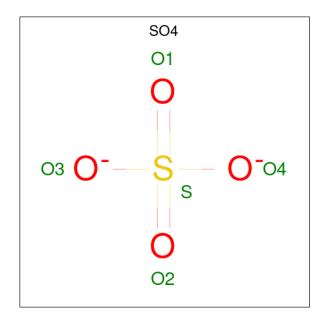
• Molecule 5 is N 7 -butyl-2-( $\{4-[(cyclobutylamino)methyl]-2-methoxyphenyl\}methyl)-2H-pyr azolo[4,3-d]pyrimidine-5,7-diamine (three-letter code: QEC) (formula: <math>C_{22}H_{31}N_7O$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
5	٨	1	Total	С	Н	N	О	91	0	
5	A	1	61	22	31	7	1	91	U	
5	D	1	Total	С	Н	N	О	91	0	
5	Б	1	61	22	31	7	1	91	0	

 $\bullet$  Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total O S 5 4 1	0	0
6	В	1	Total O S 5 4 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total O S 5 4 1	0	0

#### • Molecule 7 is water.

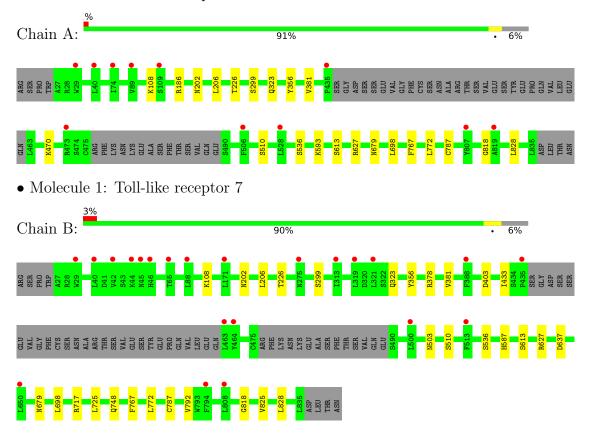
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	435	Total O 435 435	0	0
7	В	319	Total O 319 319	0	0



## 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 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 67% 33%

NAG1 NAG2 BMA3

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50% 50%





 $\bullet$  Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



 $\bullet$  Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	98.86Å 139.89Å 149.71Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.21 - 2.10	Depositor
resolution (A)	102.21 - 2.10	EDS
% Data completeness	80.1 (102.21-2.10)	Depositor
(in resolution range)	80.1 (102.21-2.10)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.26 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
D D.	0.205 , 0.238	Depositor
$R, R_{free}$	0.204 , $0.236$	DCC
$R_{free}$ test set	4728 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 53.1	EDS
L-test for twinning <sup>2</sup>	$  <  L  > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25867	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<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: QEC, SO4, NAG, BMA

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	0.41	0/6279	0.61	0/8532
1	В	0.40	0/6259	0.60	0/8509
All	All	0.41	0/12538	0.60	0/17041

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	A	6148	6068	6059	9	0
1	В	6128	6022	6013	11	0
2	С	39	34	34	0	0
3	D	28	25	25	0	0
3	Е	28	25	25	0	0
3	F	28	25	25	0	0
4	A	98	91	91	2	0
4	В	98	91	91	0	0
5	A	30	31	0	0	0
5	В	30	31	0	0	0
6	В	15	0	0	0	0



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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
7	A	435	0	0	0	0
7	В	319	0	0	1	0
All	All	13424	12443	12363	19	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 1.

All (19) 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	${f distance}({f A})$	overlap (Å)
1:A:206:LEU:O	1:A:226:THR:HG23	2.02	0.60
1:B:206:LEU:O	1:B:226:THR:HG23	2.02	0.60
1:B:767:PHE:HB3	1:B:772:LEU:HD11	1.84	0.58
1:B:510:SER:OG	1:B:536:SER:O	2.22	0.57
1:A:510:SER:OG	1:A:536:SER:O	2.22	0.57
1:A:679:ASN:HB3	4:A:907:NAG:O5	2.08	0.53
1:A:299:SER:HA	1:A:323:GLN:O	2.11	0.50
1:B:299:SER:HA	1:B:323:GLN:O	2.12	0.50
1:B:378:ARG:HD2	1:B:403:ASP:OD2	2.12	0.50
1:B:725:LEU:O	1:B:748:GLN:HG2	2.12	0.49
1:B:787:CYS:HB3	1:B:828:LEU:HD21	1.97	0.47
1:B:108:LYS:N	1:B:108:LYS:HD2	2.31	0.46
1:A:787:CYS:HB3	1:A:828:LEU:HD21	1.98	0.45
1:A:108:LYS:N	1:A:108:LYS:HD2	2.31	0.45
1:A:593:LYS:HB3	4:A:902:NAG:H81	2.00	0.43
1:A:767:PHE:HB3	1:A:772:LEU:HD11	2.00	0.42
1:A:186:ARG:HD3	1:B:637:ASP:O	2.20	0.42
1:B:587:HIS:HD2	7:B:1073:HOH:O	2.02	0.41
1:B:433:ILE:H	1:B:503:ASN:ND2	2.18	0.41

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	763/817 (93%)	718 (94%)	43 (6%)	2 (0%)	41 41
1	В	762/817 (93%)	714 (94%)	46 (6%)	2 (0%)	41 41
All	All	1525/1634 (93%)	1432 (94%)	89 (6%)	4 (0%)	41 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLY
1	В	818	GLY
1	A	381	VAL
1	В	381	VAL

#### 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	697/768~(91%)	691 (99%)	6 (1%)	78 84
1	В	691/768~(90%)	682 (99%)	9 (1%)	69 75
All	All	1388/1536 (90%)	1373 (99%)	15 (1%)	73 79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	356	TYR
1	A	470	LYS
1	A	613	SER
1	A	627	ARG
1	A	698	LEU
1	В	202	ASN
1	В	356	TYR
1	В	613	SER



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Mol	Chain	Res	Type
1	В	627	ARG
1	В	679	ASN
1	В	698	LEU
1	В	717	ARG
1	В	792	VAL
1	В	825	VAL

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	173	ASN
1	A	389	GLN
1	A	503	ASN
1	A	587	HIS
1	A	734	GLN
1	A	800	HIS
1	В	173	ASN
1	В	503	ASN
1	В	820	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)

9 monosaccharides 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	Dog	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	С	1	2,1	14,14,15	0.27	0	17,19,21	0.70	0
2	NAG	С	2	2	14,14,15	0.25	0	17,19,21	0.61	1 (5%)
2	BMA	С	3	2	11,11,12	0.23	0	15,15,17	0.37	0
3	NAG	D	1	3,1	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	Е	1	3,1	14,14,15	0.26	0	17,19,21	0.71	0
3	NAG	Е	2	3	14,14,15	0.23	0	17,19,21	0.62	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.25	0	17,19,21	0.74	1 (5%)
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.55	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1
2	BMA	С	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Е	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
3	F	1	NAG	O5-C1-C2	-2.32	107.63	111.29
3	E	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	С	2	NAG	C1-O5-C5	2.13	115.08	112.19
3	D	1	NAG	O5-C1-C2	-2.05	108.04	111.29

There are no chirality outliers.

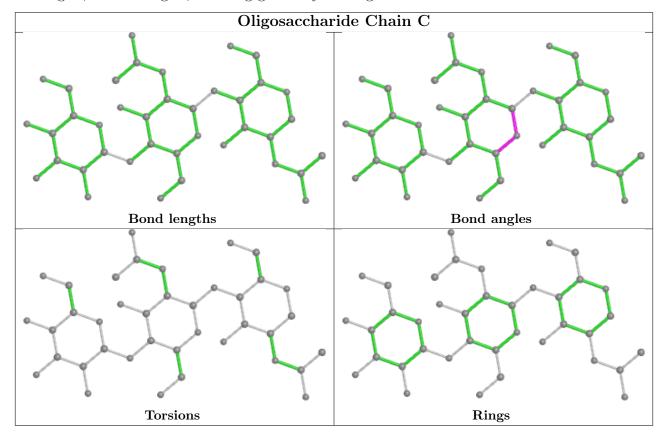
There are no torsion outliers.

There are no ring outliers.

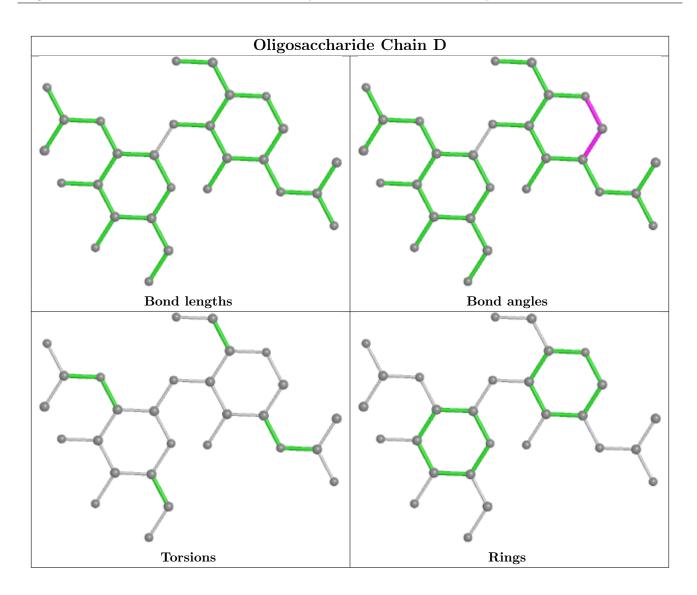
No monomer is involved in short contacts.



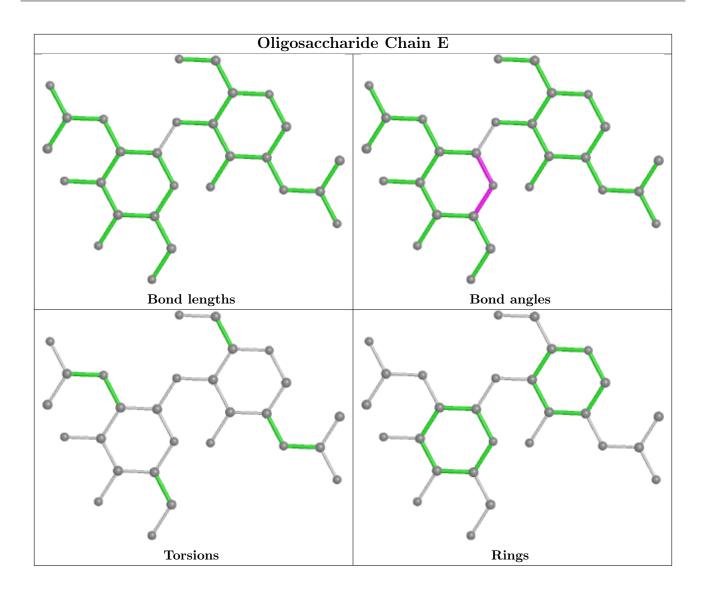
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



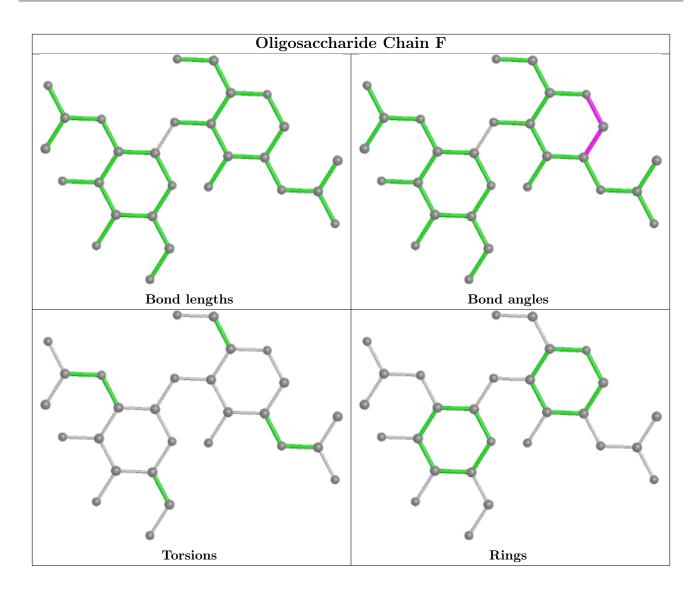












### 5.6 Ligand geometry (i)

19 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	Link	Bo	Bond lengths			Bond angles		
Moi Type Cha	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
4	NAG	A	902	1	14,14,15	0.30	0	17,19,21	0.87	1 (5%)	
4	NAG	A	904	1	14,14,15	0.31	0	17,19,21	0.47	0	
4	NAG	В	905	1	14,14,15	0.36	0	17,19,21	0.87	1 (5%)	



Mol	Type	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
WIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	В	910	_	4,4,4	0.16	0	6,6,6	0.07	0
4	NAG	A	906	1	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
4	NAG	В	906	1	14,14,15	0.28	0	17,19,21	0.94	1 (5%)
4	NAG	В	903	1	14,14,15	0.26	0	17,19,21	1.00	1 (5%)
4	NAG	В	907	1	14,14,15	0.34	0	17,19,21	0.92	1 (5%)
6	SO4	В	909	-	4,4,4	0.14	0	6,6,6	0.09	0
4	NAG	В	901	1	14,14,15	0.28	0	17,19,21	0.85	2 (11%)
5	QEC	В	908	-	30,33,33	0.75	1 (3%)	33,45,45	1.40	4 (12%)
4	NAG	В	902	1	14,14,15	0.29	0	17,19,21	0.66	0
4	NAG	В	904	1	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
4	NAG	A	901	1	14,14,15	0.27	0	17,19,21	0.84	2 (11%)
4	NAG	A	903	1	14,14,15	0.27	0	17,19,21	0.53	0
4	NAG	A	907	1	14,14,15	0.42	0	17,19,21	0.55	0
5	QEC	A	908	-	30,33,33	0.79	1 (3%)	33,45,45	1.39	4 (12%)
6	SO4	В	911	-	4,4,4	0.16	0	6,6,6	0.07	0
4	NAG	A	905	1	14,14,15	0.27	0	17,19,21	0.55	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	2/6/23/26	0/1/1/1
4	NAG	В	905	1	-	0/6/23/26	0/1/1/1
4	NAG	В	907	1	-	1/6/23/26	0/1/1/1
5	QEC	A	908	-	-	5/14/22/22	0/4/4/4
5	QEC	В	908	-	-	5/14/22/22	0/4/4/4
4	NAG	В	902	1	-	0/6/23/26	0/1/1/1
4	NAG	В	904	1	-	0/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	В	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	NAG	В	903	1	-	0/6/23/26	0/1/1/1
4	NAG	В	901	1	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
5	A	908	QEC	C4-C7	3.34	1.47	1.40
5	В	908	QEC	C4-C7	2.93	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
5	A	908	QEC	C4-N4-N2	4.97	115.34	111.45
5	В	908	QEC	C6-C18-N4	-4.16	106.06	112.17
4	В	903	NAG	O5-C1-C2	-3.98	105.00	111.29
5	В	908	QEC	C4-N4-N2	3.92	114.52	111.45
5	A	908	QEC	C6-C18-N4	-3.71	106.71	112.17
4	В	906	NAG	O5-C1-C2	-3.59	105.62	111.29
5	В	908	QEC	C14-C15-N7	-3.17	111.36	118.07
4	A	902	NAG	O5-C1-C2	-2.83	106.81	111.29
4	В	905	NAG	C1-O5-C5	2.68	115.82	112.19
4	A	906	NAG	C1-O5-C5	2.59	115.70	112.19
4	В	907	NAG	O5-C1-C2	-2.55	107.25	111.29
5	В	908	QEC	C13-C15-N7	-2.50	112.76	118.07
5	A	908	QEC	C14-C15-N7	-2.50	112.78	118.07
4	В	901	NAG	O5-C1-C2	-2.22	107.79	111.29
4	A	901	NAG	O5-C1-C2	-2.20	107.82	111.29
4	В	901	NAG	C1-O5-C5	2.13	115.07	112.19
4	A	901	NAG	C1-O5-C5	2.06	114.98	112.19
5	A	908	QEC	C13-C15-N7	-2.03	113.77	118.07
4	В	904	NAG	O5-C1-C2	-2.03	108.09	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	908	QEC	C8-C10-N6-C22
5	В	908	QEC	C8-C10-N6-C22
5	A	908	QEC	C5-C19-N7-C15
5	A	908	QEC	N3-C10-N6-C22
5	В	908	QEC	N3-C10-N6-C22
5	В	908	QEC	C5-C19-N7-C15
5	A	908	QEC	C21-C22-N6-C10
4	A	904	NAG	C4-C5-C6-O6
5	В	908	QEC	C21-C22-N6-C10
5	A	908	QEC	N4-C18-C6-C2
5	В	908	QEC	N4-C18-C6-C2



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Mol	Chain	Res	Type	Atoms
4	В	907	NAG	C1-C2-N2-C7
4	A	904	NAG	O5-C5-C6-O6

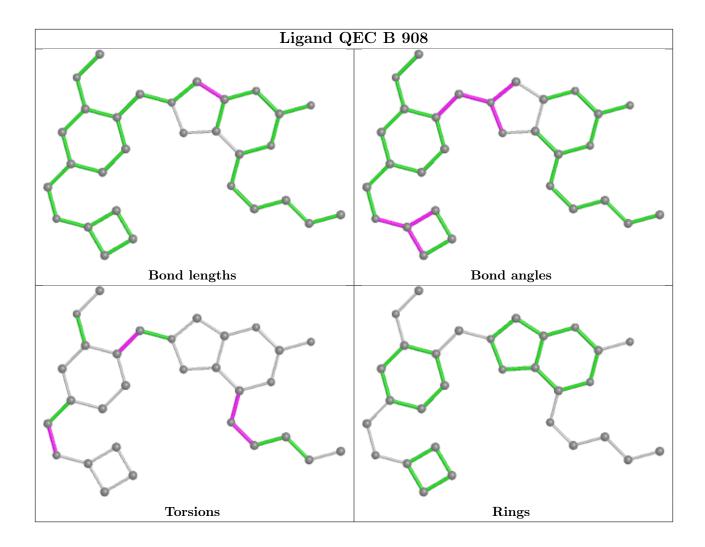
There are no ring outliers.

2 monomers are involved in 2 short contacts:

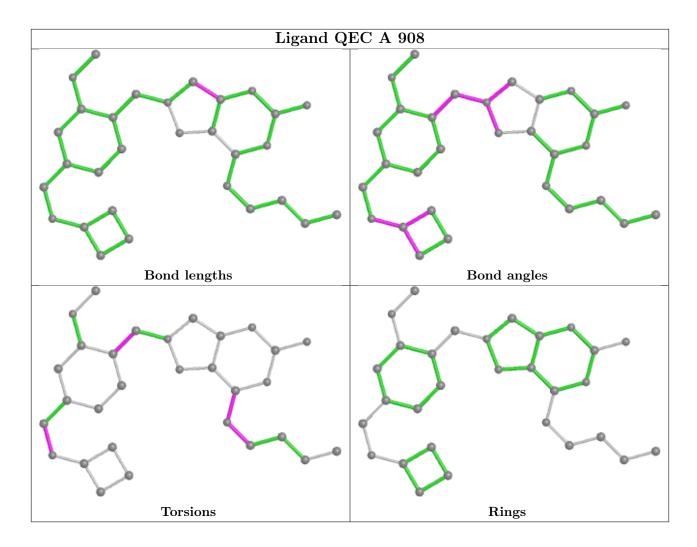
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	NAG	1	0
4	A	907	NAG	1	0

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	$OWAB(Å^2)$	Q<0.9
1	A	768/817 (94%)	0.30	11 (1%) 75 78	36, 52, 72, 89	0
1	В	768/817 (94%)	0.45	22 (2%) 51 57	41, 64, 80, 104	0
All	All	1536/1634 (94%)	0.38	33 (2%) 63 68	36, 58, 78, 104	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	42	VAL	4.9
1	A	109	SER	4.3
1	В	29	TRP	3.9
1	В	313	ILE	3.8
1	В	435	PRO	3.5
1	В	40	LEU	3.3
1	A	506	PHE	3.0
1	В	275	ASN	2.8
1	В	45	ASN	2.8
1	В	463	LEU	2.7
1	В	513	PHE	2.7
1	A	819	ALA	2.7
1	A	89	VAL	2.6
1	В	65	THR	2.6
1	В	808	LEU	2.6
1	A	435	PRO	2.6
1	В	464	TYR	2.6
1	В	44	LYS	2.6
1	В	650	LEU	2.5
1	В	319	LEU	2.5
1	A	807	TYR	2.4
1	A	29	TRP	2.3
1	В	171	LEU	2.2
1	В	500	LEU	2.2



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Mol	Chain	Res	Type	RSRZ
1	A	528	LEU	2.2
1	A	74	ILE	2.2
1	В	46	HIS	2.2
1	A	40	LEU	2.1
1	В	88	LEU	2.1
1	В	388	PHE	2.1
1	A	473	ARG	2.1
1	В	321	LEU	2.0
1	В	794	PHE	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.

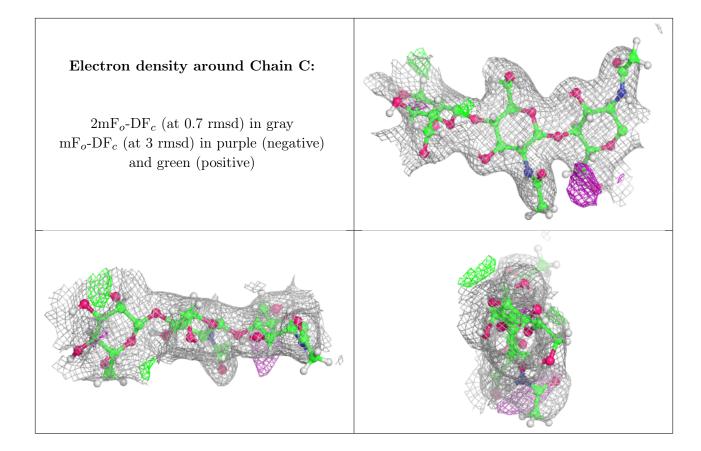
### 6.3 Carbohydrates (i)

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.

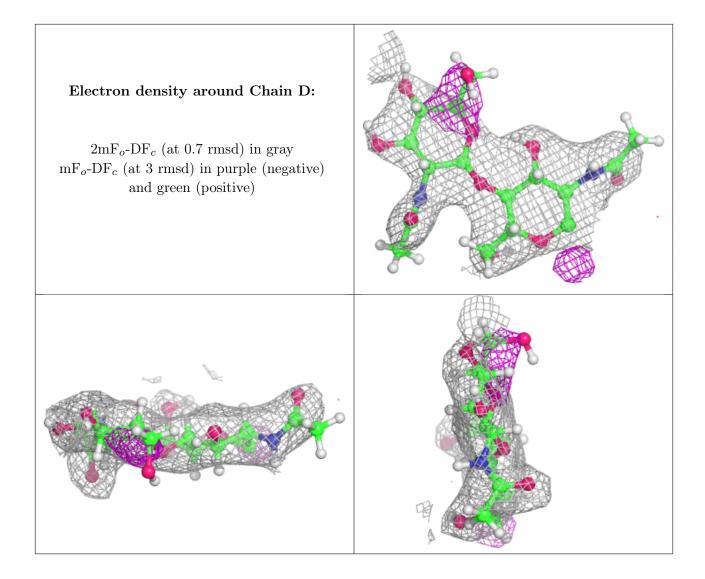
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	NAG	D	2	14/15	0.76	0.32	84,86,103,104	13
2	BMA	С	3	11/12	0.82	0.16	88,91,119,120	10
3	NAG	F	2	14/15	0.83	0.27	96,98,127,128	13
3	NAG	D	1	14/15	0.90	0.17	75,78,92,93	12
2	NAG	С	2	14/15	0.91	0.09	78,83,105,106	12
3	NAG	F	1	14/15	0.92	0.13	89,92,118,118	12
3	NAG	Е	2	14/15	0.93	0.09	73,76,95,96	13
2	NAG	С	1	14/15	0.96	0.14	66,71,88,89	12
3	NAG	Е	1	14/15	0.97	0.12	65,69,85,85	12

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

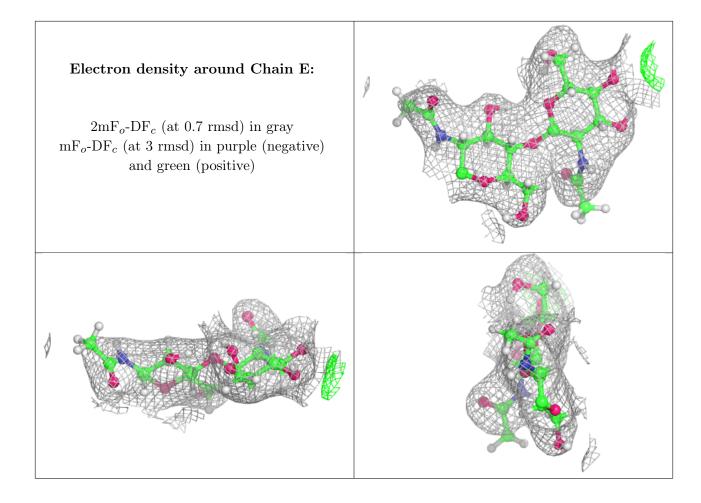




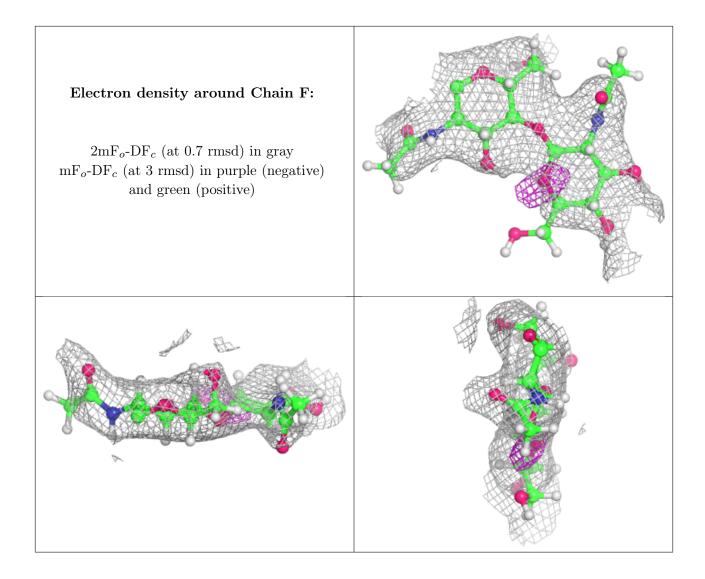












### 6.4 Ligands (i)

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.

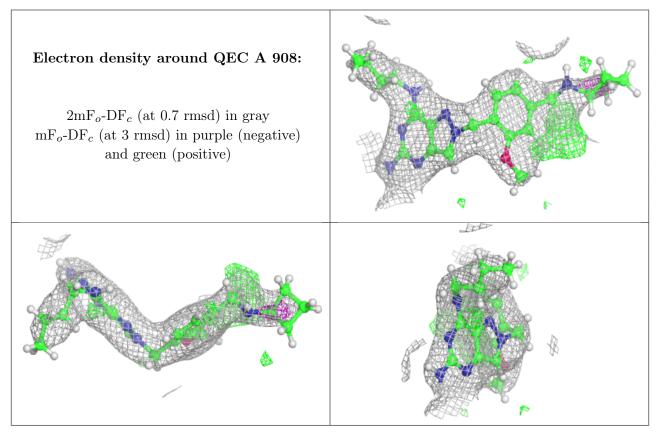
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
4	NAG	В	907	14/15	0.59	0.36	99,102,141,143	13
4	NAG	В	905	14/15	0.67	0.24	93,95,132,133	13
4	NAG	A	907	14/15	0.69	0.23	75,77,84,85	13
6	SO4	В	910	5/5	0.76	0.18	156,156,156,156	0
6	SO4	В	911	5/5	0.81	0.15	157,157,157,157	0
4	NAG	В	906	14/15	0.82	0.27	85,88,111,112	13
4	NAG	A	906	14/15	0.86	0.16	75,77,103,103	13
6	SO4	В	909	5/5	0.90	0.53	155,155,155,155	0
4	NAG	В	903	14/15	0.92	0.10	84,86,119,120	13



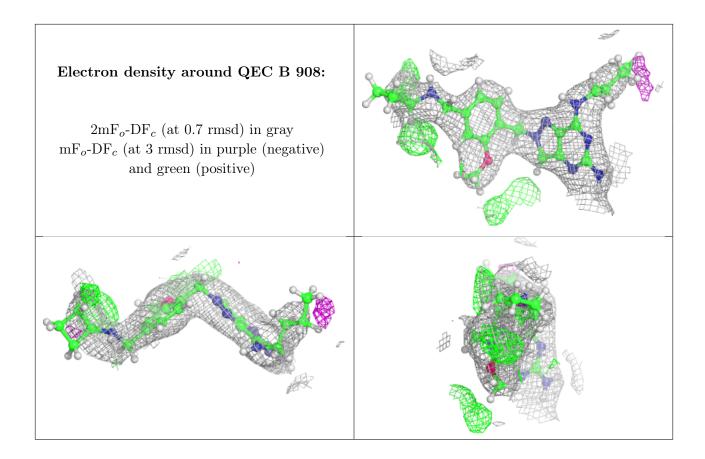
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
5	QEC	A	908	30/30	0.92	0.17	55,67,85,85	31
5	QEC	В	908	30/30	0.92	0.17	52,63,84,85	31
4	NAG	A	903	14/15	0.93	0.16	63,66,78,80	13
4	NAG	A	905	14/15	0.94	0.09	75,78,106,108	13
4	NAG	В	904	14/15	0.94	0.12	80,81,117,119	13
4	NAG	A	902	14/15	0.94	0.11	64,67,86,88	13
4	NAG	A	904	14/15	0.94	0.09	69,71,97,99	13
4	NAG	В	902	14/15	0.94	0.13	73,75,103,104	13
4	NAG	A	901	14/15	0.95	0.15	48,53,59,61	13
4	NAG	В	901	14/15	0.96	0.12	56,59,67,68	13

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.

