

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

#### Nov 27, 2023 – 01:43 PM JST

PDB ID	:	7XYD
Title	:	Crystal structure of TMPRSS2 in complex with Nafamostat
Authors	:	Wang, H.; Liu, X.; Duan, Y.; Liu, X.; Sun, L.; Yang, H.
Deposited on		
Resolution	:	2.58  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:

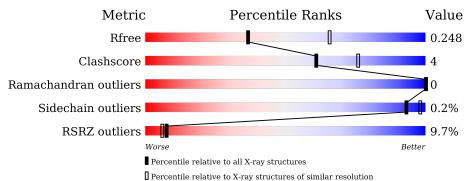
Xtriage (Phenix) EDS buster-report Percentile statistics	: : :	20191225.v01 (using entries in the PDB archive December 25th 2019)
-	:	
CCP4 Ideal geometry (proteins)		7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		

# 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 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3676 (2.60-2.56)
Clashscore	141614	4049(2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	146	83%	5%	12%
1	В	146	64% 21%	•	14%
2	С	249	4% 92%		5% •
2	D	249	3% 		9% •



В

В

В

В

251

252

253

254

ASP

ASP

ASP

LYS

#### 7XYD

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	129	Total	С	Ν	0	S	0	0	0
1	I A	129	980	598	175	196	11	0		
1	1 B	125	Total	С	Ν	0	S	0	0	0
			948	578	171	186	13		U	

• Molecule 1 is a protein called Transmembrane protease serine 2 catalytic chain.

Chain	Residue	Modelled	Actual	Comment	Reference
А	250	ASP	SER	engineered mutation	UNP O15393
А	251	ASP	SER	engineered mutation	UNP O15393
А	252	ASP	ARG	engineered mutation	UNP 015393
А	253	ASP	GLN	engineered mutation	UNP O15393
А	254	LYS	SER	engineered mutation	UNP 015393
В	250	ASP	SER	engineered mutation	UNP O15393

SER

ARG

GLN

SER

There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Transmembrane protease serine 2 catalytic chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
0	C	242	Total	С	Ν	0	S	0	0	0
	U	242	1856	1189	312	340	15	0		
0	2 D	239	Total	С	Ν	0	S	0	1	0
			1842	1183	313	330	16	0	1	

engineered mutation

engineered mutation

engineered mutation

engineered mutation

There are 24 discrepancies between the modelled and reference sequences:

C493GLU-expression tagUNP O15393C494PHE-expression tagUNP O15393	Chain	Residue	Modelled	Actual	Comment	Reference
C 494 PHE - expression tag UNP O15393	С	493	GLU	-	expression tag	UNP O15393
	С	494	PHE	-	expression tag	UNP O15393

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<u>UNP</u> O15393

UNP 015393

UNP 015393

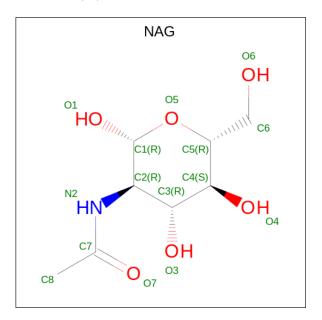
UNP 015393



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Chain	Residue	Modelled	Actual	Comment	Reference
С	495	VAL	-	expression tag	UNP O15393
С	496	GLU	-	expression tag	UNP O15393
С	497	HIS	-	expression tag	UNP O15393
С	498	HIS	-	expression tag	UNP O15393
С	499	HIS	-	expression tag	UNP O15393
С	500	HIS	-	expression tag	UNP O15393
С	501	HIS	-	expression tag	UNP O15393
С	502	HIS	-	expression tag	UNP O15393
С	503	HIS	-	expression tag	UNP O15393
С	504	HIS	-	expression tag	UNP O15393
D	493	GLU	-	expression tag	UNP O15393
D	494	PHE	-	expression tag	UNP O15393
D	495	VAL	-	expression tag	UNP O15393
D	496	GLU	-	expression tag	UNP O15393
D	497	HIS	-	expression tag	UNP O15393
D	498	HIS	-	expression tag	UNP O15393
D	499	HIS	-	expression tag	UNP O15393
D	500	HIS	-	expression tag	UNP O15393
D	501	HIS	-	expression tag	UNP O15393
D	502	HIS	-	expression tag	UNP O15393
D	503	HIS	-	expression tag	UNP O15393
D	504	HIS	-	expression tag	UNP O15393

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



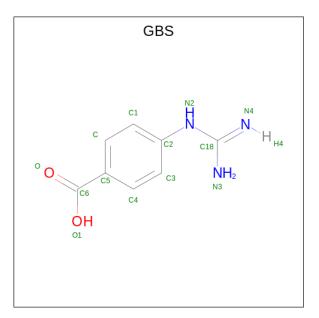


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total         C         N         O           14         8         1         5	0	0
3	В	1	Total         C         N         O           14         8         1         5	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

• Molecule 5 is 4-carbamimidamidobenzoic acid (three-letter code: GBS) (formula:  $C_8H_9N_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total         C         N         O           12         8         3         1	0	0
5	D	1	Total         C         N         O           12         8         3         1	0	0

• Molecule 6 is water.



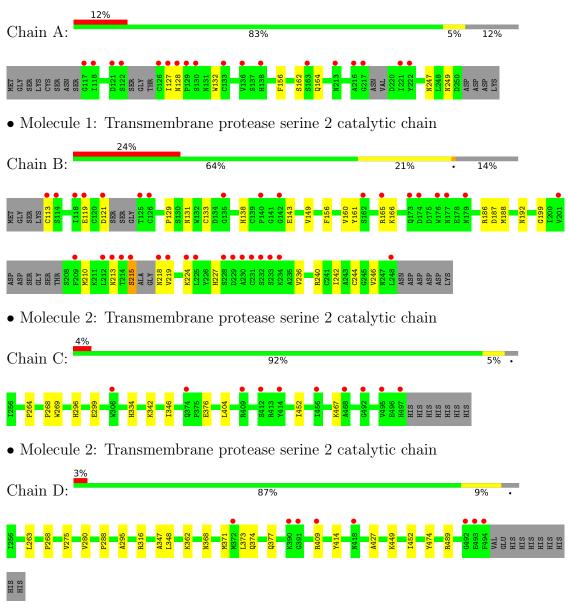
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	22	Total O 22 22	0	0
6	С	63	Total         O           63         63	0	0
6	В	10	Total         O           10         10	0	0
6	D	58	Total         O           58         58	0	0



## 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: Transmembrane protease serine 2 catalytic chain





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	49.14Å 93.20Å 93.13Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $100.60^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	39.81 - 2.58	Depositor
Resolution (A)	39.80 - 2.58	EDS
% Data completeness	98.5 (39.81-2.58)	Depositor
(in resolution range)	98.5 (39.80-2.58)	EDS
R <sub>merge</sub>	0.17	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.211 , 0.248	Depositor
$R, R_{free}$	0.211 , $0.248$	DCC
$R_{free}$ test set	2004 reflections $(7.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $41.4$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5833	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 6.02% 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: NAG, GBS, CA

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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.31	0/1000	0.53	0/1353
1	В	0.35	0/967	0.54	0/1307
2	С	0.29	0/1912	0.51	0/2616
2	D	0.31	0/1900	0.51	0/2596
All	All	0.31	0/5779	0.52	0/7872

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	А	980	0	866	7	0
1	В	948	0	830	23	0
2	С	1856	0	1752	8	0
2	D	1842	0	1771	19	0
3	А	14	0	13	0	0
3	В	14	0	13	3	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	С	12	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	12	0	0	0	0
6	А	22	0	0	0	0
6	В	10	0	0	0	0
6	С	63	0	0	0	0
6	D	58	0	0	0	0
All	All	5833	0	5245	49	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 4.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A / 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:218:ASN:HB3	1:B:224:LYS:HZ1	1.55	0.72
1:B:186:ARG:HH21	1:B:192:ASN:CG	2.01	0.64
2:C:264:PRO:HD2	2:D:263:LEU:HD13	1.80	0.63
1:B:242:ILE:HD11	2:D:288:PRO:HD3	1.81	0.61
2:D:373:LEU:HB3	2:D:377:GLN:HG3	1.80	0.61
1:B:121:ASP:HB2	1:B:143:GLU:HG2	1.83	0.61
1:B:156:PHE:HE1	2:D:452:ILE:HD13	1.69	0.58
2:C:334:HIS:HB2	2:C:346:ILE:HG23	1.86	0.57
1:B:187:ASP:HA	2:D:489:ARG:NH1	2.20	0.57
1:B:246:VAL:HG23	2:D:362:LYS:HD3	1.87	0.57
2:C:296:HIS:HA	2:C:299:GLU:HG3	1.88	0.56
1:A:128:ASN:OD1	1:A:128:ASN:N	2.40	0.54
1:B:149:VAL:HG11	1:B:187:ASP:HB2	1.90	0.54
1:B:113:CYS:SG	1:B:119:GLU:HG3	2.50	0.52
1:A:162:SER:OG	1:A:164:GLN:CD	2.48	0.52
1:B:199:GLY:HA2	1:B:236:VAL:O	2.10	0.51
2:D:275:VAL:HB	2:D:280:VAL:HG21	1.91	0.51
1:B:215:SER:HB2	3:B:301:NAG:H5	1.93	0.50
1:A:127:ILE:HD11	1:A:132:TRP:HB2	1.93	0.50
2:D:409:ARG:NH1	2:D:414:TYR:OH	2.45	0.50
1:A:162:SER:OG	1:A:164:GLN:NE2	2.45	0.49
2:D:368:ASN:O	2:D:371:MET:HG2	2.11	0.49
1:B:160:VAL:HG12	1:B:210:MET:HG3	1.94	0.48
1:B:240:ARG:HH21	1:B:244:CYS:H	1.60	0.48
1:A:156:PHE:HE1	2:C:452:ILE:HD13	1.79	0.48
1:A:247:ASN:HD21	1:A:249:ASN:ND2	2.13	0.46
2:D:427:ALA:HB3	2:D:474:TYR:CE1	2.50	0.46
1:B:129:PRO:HB2	1:B:166:LYS:HD2	1.97	0.46



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:CYS:HB2	1:B:161:TYR:HD2	1.82	0.45
1:B:213:ASN:OD1	3:B:301:NAG:N2	2.51	0.43
2:D:268:PRO:HB2	2:D:362:LYS:H	1.82	0.43
2:D:374:GLN:H	2:D:377:GLN:HG2	1.82	0.43
1:B:219:VAL:HG22	1:B:224:LYS:HE2	1.99	0.43
2:D:268:PRO:HB2	2:D:362:LYS:N	2.34	0.43
2:C:376:GLU:HA	2:C:404:LEU:O	2.19	0.43
1:B:165:ARG:HH21	1:B:227:HIS:CD2	2.37	0.43
2:D:295:ALA:HA	2:D:347:ALA:HB2	2.00	0.42
1:B:156:PHE:CE1	2:D:452:ILE:HD13	2.52	0.42
2:C:467:LYS:HA	2:C:467:LYS:HD3	1.91	0.41
1:B:149:VAL:HG13	1:B:188:MET:HG2	2.02	0.41
2:C:342:LYS:HD3	2:C:342:LYS:HA	1.87	0.41
2:C:268:PRO:HG2	2:C:269:TRP:CE3	2.55	0.41
1:B:165:ARG:NH2	1:B:227:HIS:NE2	2.68	0.41
1:B:215:SER:HB2	3:B:301:NAG:C5	2.51	0.41
2:D:348:LEU:HD23	2:D:348:LEU:HA	1.88	0.41
1:A:249:ASN:O	2:D:316:ARG:NH2	2.54	0.41
1:B:131:ASN:HB3	1:B:138:HIS:CE1	2.55	0.41
2:D:371:MET:O	2:D:449:LYS:NZ	2.51	0.40
2:D:374:GLN:H	2:D:377:GLN:CG	2.34	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	123/146~(84%)	120 (98%)	3~(2%)	0	100	100
1	В	117/146~(80%)	113 (97%)	4 (3%)	0	100	100
2	С	240/249~(96%)	232 (97%)	8 (3%)	0	100	100
2	D	238/249~(96%)	230 (97%)	8 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	718/790~(91%)	695~(97%)	23 (3%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	106/127~(84%)	106 (100%)	0	100 100
1	В	103/127~(81%)	102 (99%)	1 (1%)	76 89
2	С	195/210~(93%)	195 (100%)	0	100 100
2	D	195/210~(93%)	195 (100%)	0	100 100
All	All	599/674~(89%)	598 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	215	SER

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	249	ASN
1	В	115	ASN
1	В	131	ASN
1	В	218	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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).

Mol	Mol Type Chain Bee		Res	Link	Bond lengths			Bond angles		
	Mol Type Chain	nes Lin		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
5	GBS	D	601	2	12,12,13	0.91	0	15,15,17	0.62	0
5	GBS	С	601	2	12,12,13	0.88	0	15,15,17	0.52	0
3	NAG	В	301	1	14,14,15	0.45	0	17,19,21	0.67	0
3	NAG	А	301	1	14,14,15	0.39	0	17,19,21	0.56	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
5	GBS	D	601	2	-	3/6/6/8	0/1/1/1
5	GBS	С	601	2	-	3/6/6/8	0/1/1/1
3	NAG	В	301	1	-	4/6/23/26	0/1/1/1
3	NAG	А	301	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	В	301	NAG	C8-C7-N2-C2
3	В	301	NAG	O7-C7-N2-C2
3	А	301	NAG	C4-C5-C6-O6
3	А	301	NAG	O5-C5-C6-O6
3	В	301	NAG	O5-C5-C6-O6
3	В	301	NAG	C4-C5-C6-O6
3	А	301	NAG	C8-C7-N2-C2
5	D	601	GBS	C-C5-C6-O
3	А	301	NAG	O7-C7-N2-C2
5	D	601	GBS	C4-C5-C6-O
5	С	601	GBS	N3-C18-N2-C2
5	D	601	GBS	N3-C18-N2-C2
5	С	601	GBS	C4-C5-C6-O
5	С	601	GBS	C-C5-C6-O

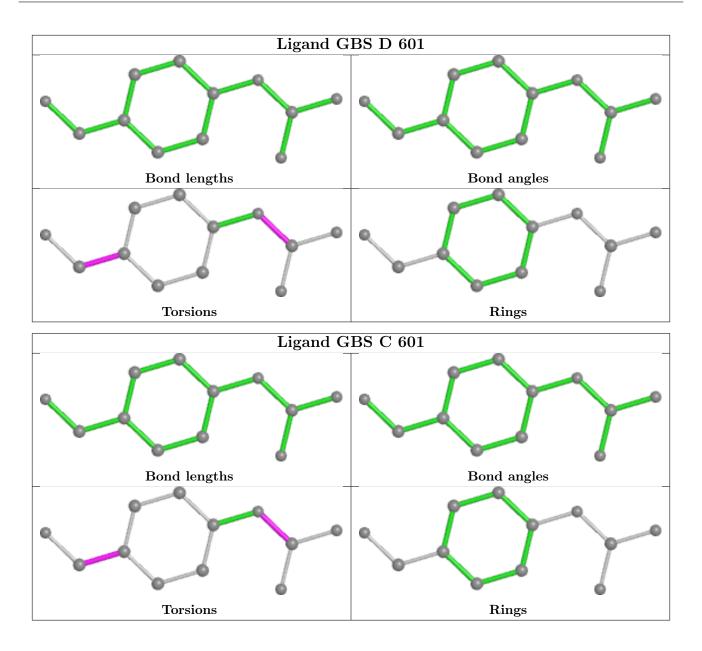
There are no ring outliers.

1 monomer is involved in 3 short contacts:

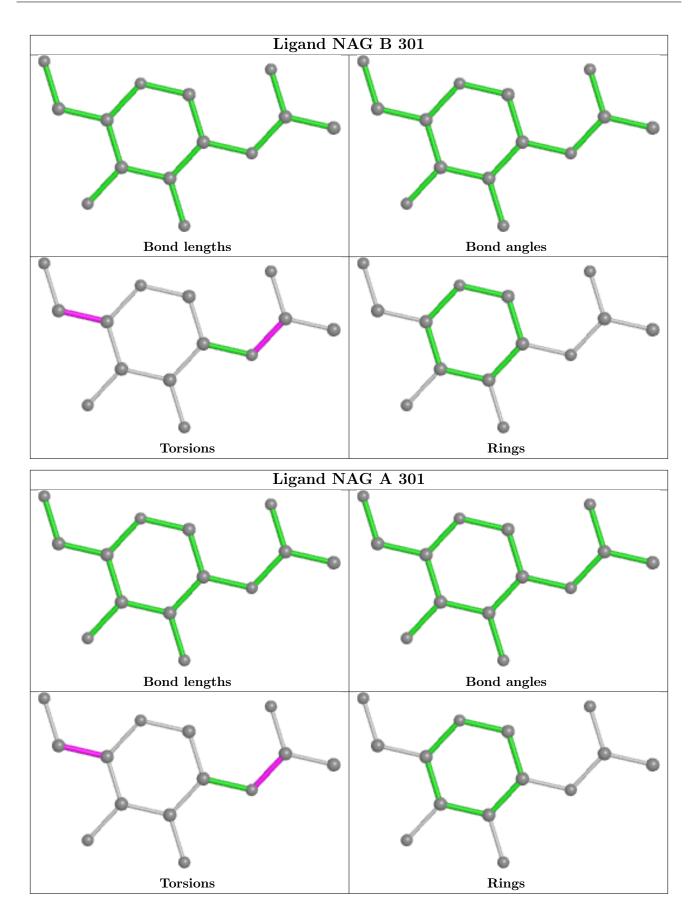
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	301	NAG	3	0

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 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	$OWAB(Å^2)$	Q<0.9
1	А	129/146~(88%)	0.67	18 (13%) 2 2	30, 43, 77, 85	0
1	В	125/146~(85%)	1.50	35 (28%) 0 0	43, 65, 88, 98	0
2	С	242/249~(97%)	0.34	10 (4%) 37 33	26, 35, 51, 82	0
2	D	239/249~(95%)	0.47	8 (3%) 46 42	28, 39, 57, 84	0
All	All	735/790~(93%)	0.64	71 (9%) 7 6	26, 40, 77, 98	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	129	PRO	6.2
2	D	494	PHE	5.5
1	В	230	ALA	5.3
1	В	218	ASN	5.0
1	А	122	SER	4.9
1	В	201	VAL	4.9
1	А	130	SER	4.8
1	В	114	SER	4.6
1	В	173	GLN	4.4
1	В	213	ASN	4.4
2	С	414	TYR	4.3
1	В	233	SER	3.9
1	В	212	LEU	3.8
1	В	232	SER	3.8
1	В	179	ASN	3.7
1	В	229	ASP	3.7
1	В	219	VAL	3.7
2	D	372	MET	3.7
1	В	176	TRP	3.6
1	А	127	ILE	3.6
1	А	126	CYS	3.5



Mol	Chain	Res	ous pageType	RSRZ
1	В	234	LYS	3.5
1	B	228	SER	3.4
1	B	231	CYS	3.3
1	B	113	CYS	3.2
1	A	138	HIS	3.2
1	В	174	ASP	3.1
1	B	118	ILE	3.1
1	A	213	ASN	3.1
1	В	224	LYS	3.0
1	В	125	THR	3.0
1	В	121	ASP	2.9
1	В	209	PHE	2.8
2	D	493	GLU	2.8
1	А	216	ALA	2.7
2	С	412	SER	2.7
1	А	118	ILE	2.7
1	В	215	SER	2.7
2	С	409	ARG	2.7
2	С	497	HIS	2.7
1	В	119	GLU	2.6
1	В	214	THR	2.6
2	D	409	ARG	2.6
1	В	248	LEU	2.5
1	А	117	GLY	2.5
1	В	140	PRO	2.5
2	D	418	ASN	2.5
1	А	163	SER	2.4
1	В	126	CYS	2.4
2	С	374	GLN	2.4
1	А	222	TYR	2.4
2	С	456	ILE	2.3
1	В	165	ARG	2.3
2	С	495	VAL	2.3
1	А	221	ILE	2.3
2	C A	492	GLY	2.3
1		217	GLY	2.2
2	С	306	TRP	2.2
2	D	391	GLY	2.2
1	В	135	GLY	2.2
1	В	162	SER	2.2
2	С	468	ALA	2.2
1	А	128	ASN	2.2



Mol	Chain	Res	Type	RSRZ
2	D	492	GLY	2.1
1	А	133	CYS	2.1
1	А	121	ASP	2.1
1	А	136	VAL	2.1
1	В	225	LEU	2.1
1	В	142	GLY	2.1
1	В	177	ASN	2.0
2	D	390	LYS	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.

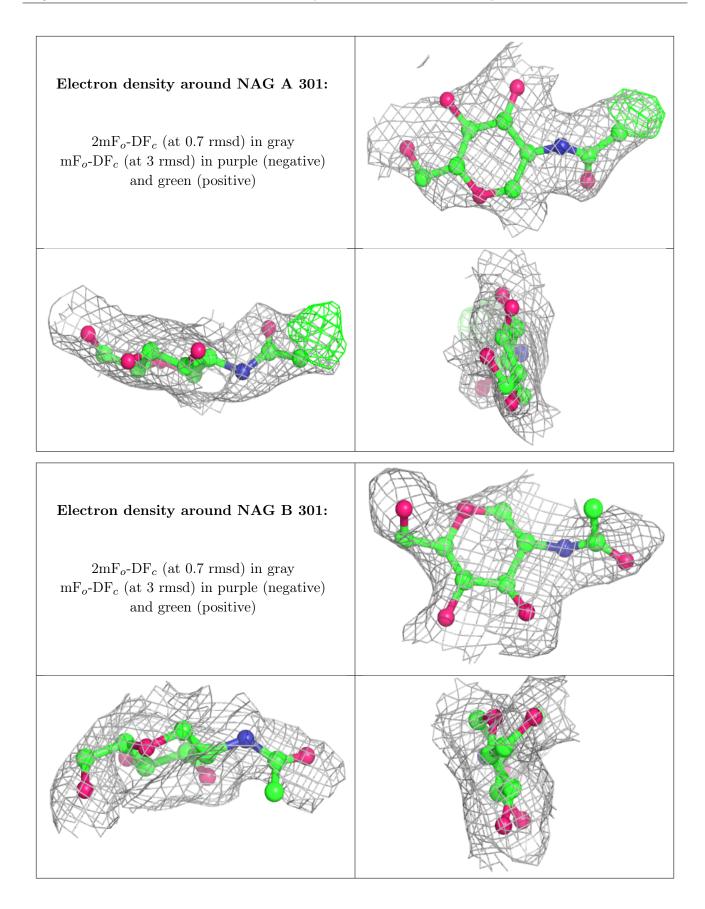
#### 6.4 Ligands (i)

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.

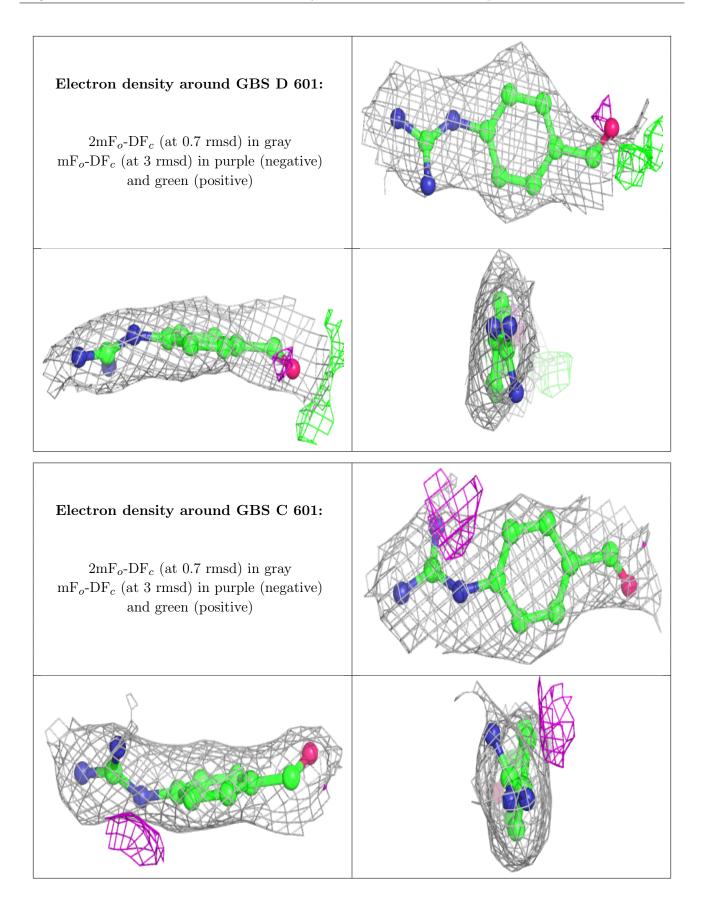
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
3	NAG	А	301	14/15	0.67	0.37	61,80,85,89	0
3	NAG	В	301	14/15	0.76	0.28	65,77,81,83	0
5	GBS	D	601	12/13	0.89	0.23	40,46,56,72	0
5	GBS	С	601	12/13	0.92	0.19	34,41,42,43	0
4	CA	В	302	1/1	0.94	0.09	67,67,67,67	0
4	CA	А	302	1/1	0.97	0.13	$65,\!65,\!65,\!65$	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.

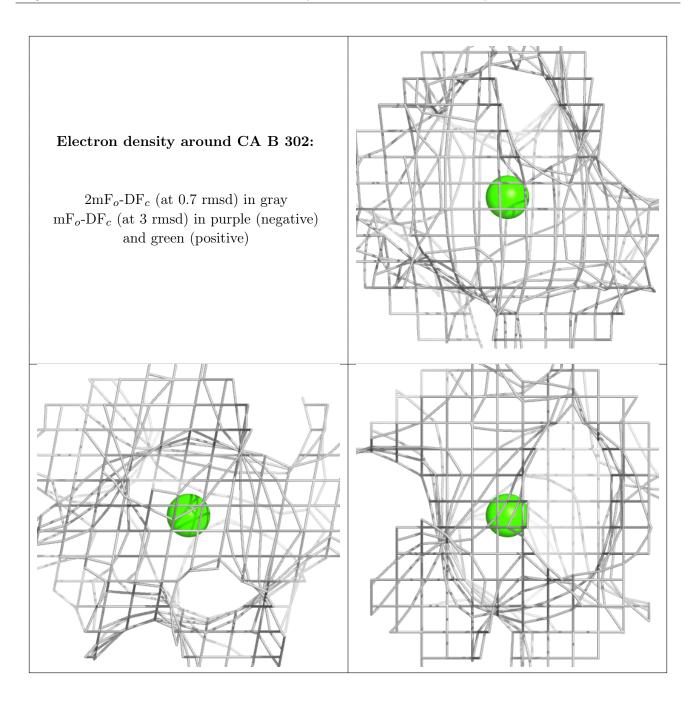




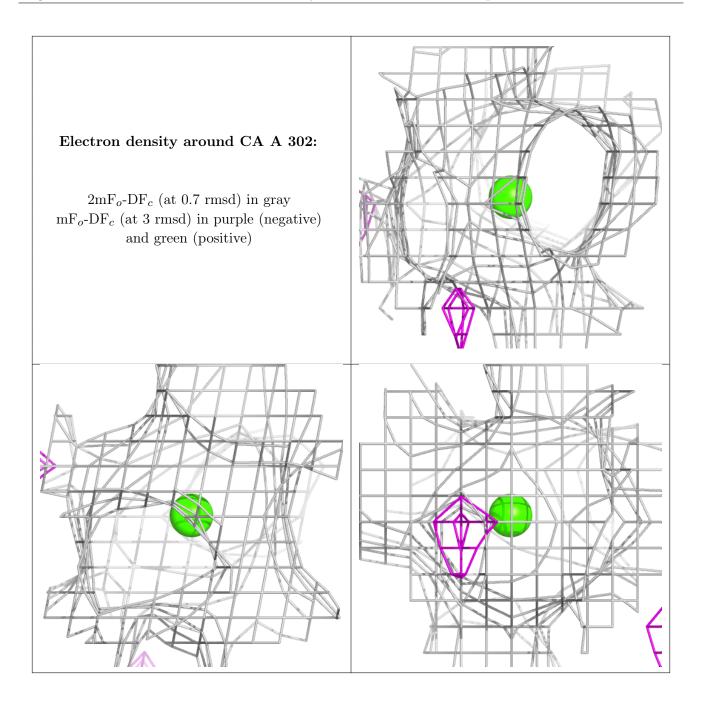












## 6.5 Other polymers (i)

There are no such residues in this entry.

