

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

Nov 21, 2023 – 02:37 AM JST

PDB ID : 7EKE

Title: Structure of SARS-CoV-2 spike receptor-binding domain F486L mutation com-

plexed with human ACE2

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Deposited on : 2021-04-05

Resolution : 2.70 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)

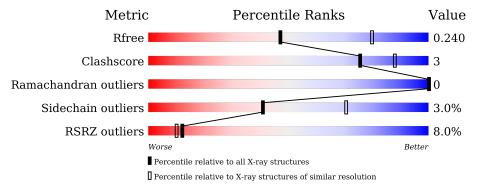
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.70 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	603	90%			8%		
2	В	229	72%	11%		15%	-	



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6465 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	596	Total 4862	C 3111	N 805	O 917	S 29	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1

• Molecule 2 is a protein called Spike protein S1.

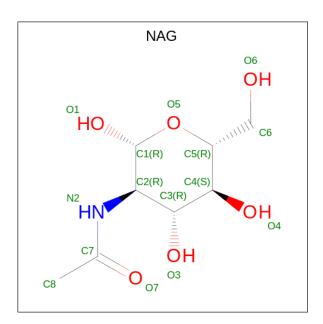
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	195	Total	С	N	0	S	0	1	0
			1546	990	258	290	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
В	486	LEU	PHE	engineered mutation	UNP P0DTC2
В	542	HIS	-	expression tag	UNP P0DTC2
В	543	HIS	-	expression tag	UNP P0DTC2
В	544	HIS	-	expression tag	UNP P0DTC2
В	545	HIS	-	expression tag	UNP P0DTC2
В	546	HIS	-	expression tag	UNP P0DTC2
В	547	HIS	-	expression tag	UNP P0DTC2

• 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	A	1	Total C N O	0	0	
	11	1	14 8 1 5	· ·		
2	Λ	1	Total C N O	0	0	
3	Α	1	14 8 1 5	0	U	
2	Λ	1	Total C N O	0	0	
3	Α	1	14 8 1 5	0		
2	D	1	Total C N O	0	0	
3	Ъ	1	14 8 1 5	0	U	

 $\bullet$  Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

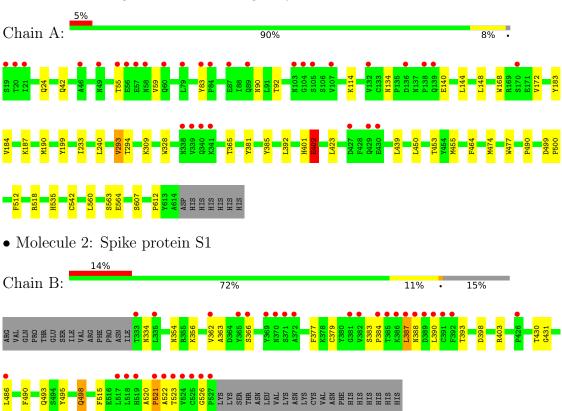
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0



# 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: Angiotensin-converting enzyme 2





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	104.32Å 104.32Å 228.37Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.50 - 2.70	Depositor
Resolution (A)	47.44 - 2.70	EDS
% Data completeness	98.8 (20.50-2.70)	Depositor
(in resolution range)	98.8 (47.44-2.70)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.58 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
D D.	0.212 , 0.241	Depositor
$R, R_{free}$	0.210 , 0.240	DCC
$R_{free}$ test set	1725 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 29.9	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% 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: ZN, NAG

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	Bo	nd lengths	Bond angles		
IVIOI	$egin{array}{c c} oldsymbol{\mathrm{Mol}} & \mathrm{Chain} & \mathrm{RM} \end{array}$		# Z  > 5	RMSZ	# Z >5	
1	A	0.35	$2/4999 \ (0.0\%)$	0.45	0/6792	
2	В	0.37	1/1592 (0.1%)	0.49	0/2169	
All	All	0.35	3/6591 (0.0%)	0.46	0/8961	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	A	402	GLU	CD-OE2	-9.56	1.15	1.25
2	В	490	PHE	C-N	7.91	1.49	1.34
1	A	402	GLU	CD-OE1	-6.29	1.18	1.25

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	4862	0	4636	25	0
2	В	1546	0	1469	18	0
3	A	42	0	39	0	0
3	В	14	0	13	0	0
4	A	1	0	0	0	0
All	All	6465	0	6157	39	0



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 3.

All (39) 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:42:GLN:HE22	2:B:498[A]:GLN:HE22	1.27	0.82
1:A:42:GLN:NE2	2:B:498[A]:GLN:HE22	1.82	0.77
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.70	0.73
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.74	0.69
2:B:362:VAL:HG13	2:B:526:GLY:HA2	1.73	0.69
2:B:520:ALA:HB1	2:B:521:PRO:HD2	1.77	0.64
1:A:42:GLN:NE2	2:B:498[A]:GLN:NE2	2.50	0.58
1:A:42:GLN:HE22	2:B:498[A]:GLN:NE2	2.00	0.57
2:B:334:ASN:O	2:B:362:VAL:N	2.39	0.55
2:B:393:THR:HA	2:B:522:ALA:HA	1.87	0.55
2:B:521:PRO:HB2	2:B:523:THR:HG23	1.88	0.55
2:B:383:SER:H	2:B:387:LEU:HD12	1.71	0.55
1:A:134:ASN:OD1	1:A:140:GLU:HB3	2.10	0.52
1:A:90:ASN:OD1	1:A:92:THR:HG22	2.13	0.49
1:A:294:THR:HG23	1:A:365:THR:HA	1.95	0.47
1:A:187:LYS:HD2	1:A:199:TYR:CZ	2.51	0.46
2:B:379:CYS:HB2	2:B:384:PRO:HD3	1.98	0.46
1:A:560:LEU:HD22	1:A:564:GLU:HG3	1.98	0.46
1:A:184:VAL:HG22	1:A:464:PHE:HE1	1.80	0.46
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.98	0.45
2:B:354:ASN:O	2:B:398:ASP:HA	2.18	0.44
1:A:55:THR:O	1:A:59:VAL:HG23	2.18	0.44
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.88	0.44
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.53	0.43
1:A:474:MET:HE1	1:A:499:ASP:HB2	2.00	0.43
2:B:403:ARG:HG2	2:B:495:TYR:CE1	2.54	0.42
1:A:233:ILE:HD13	1:A:450:LEU:HD13	2.01	0.42
1:A:477:TRP:CZ3	1:A:500:PRO:HB3	2.55	0.42
1:A:535:HIS:CE1	1:A:542:CYS:HA	2.54	0.42
1:A:42:GLN:HA	1:A:42:GLN:OE1	2.19	0.41
1:A:24:GLN:HB3	1:A:83:TYR:HE1	1.85	0.41
2:B:431:GLY:HA2	2:B:515:PHE:CD2	2.55	0.41
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.56	0.41
2:B:388:ASN:OD1	2:B:388:ASN:N	2.49	0.41
1:A:293:VAL:HG22	1:A:423:LEU:HB3	2.03	0.41
2:B:383:SER:HB2	2:B:387:LEU:HG	2.03	0.41
1:A:392:LEU:HD13	1:A:563:SER:HA	2.02	0.40

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:453:THR:HG23	1:A:512:PHE:CD2	2.56	0.40
2:B:363:ALA:H	2:B:526:GLY:HA3	1.87	0.40

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	594/603 (98%)	586 (99%)	8 (1%)	0	100	100
2	В	194/229~(85%)	183 (94%)	11 (6%)	0	100	100
All	All	788/832 (95%)	769 (98%)	19 (2%)	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	A	526/533 (99%)	514 (98%)	12 (2%)	50 78
2	В	169/202 (84%)	159 (94%)	10 (6%)	19 43
All	All	$695/735 \; (95\%)$	673 (97%)	22 (3%)	41 68

All (22) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	114	LYS
1	A	183	TYR
1	A	190	MET
1	A	240	LEU
1	A	293	VAL
1	A	381	TYR
1	A	385	TYR
1	A	401	HIS
1	A	402	GLU
1	A	439	LEU
1	A	455	MET
1	A	607	SER
2	В	356	LYS
2	В	366	SER
2	В	377	PHE
2	В	387	LEU
2	В	430	THR
2	В	486	LEU
2	В	493	GLN
2	В	498[A]	GLN
2	В	498[B]	GLN
2	В	521	PRO

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

Mol	Chain	Res	Type
1	A	81	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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is 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	Type Chain		Dog I	s Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	701	1	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
3	NAG	A	703	1	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	В	601	2	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	A	702	1	14,14,15	0.35	0	17,19,21	0.62	1 (5%)

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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	В	601	2	-	2/6/23/26	0/1/1/1
3	NAG	A	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
3	A	701	NAG	C1-O5-C5	2.36	115.39	112.19
3	A	702	NAG	C1-O5-C5	2.18	115.14	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NAG	O5-C5-C6-O6
3	A	702	NAG	C4-C5-C6-O6

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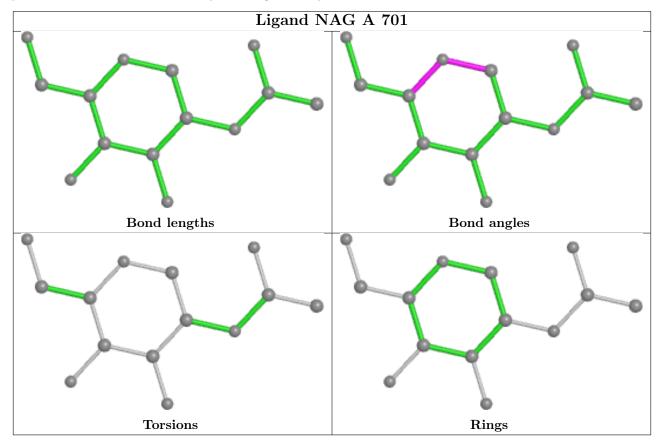
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Mol	Chain	Res	Type	Atoms
3	В	601	NAG	C4-C5-C6-O6
3	В	601	NAG	O5-C5-C6-O6

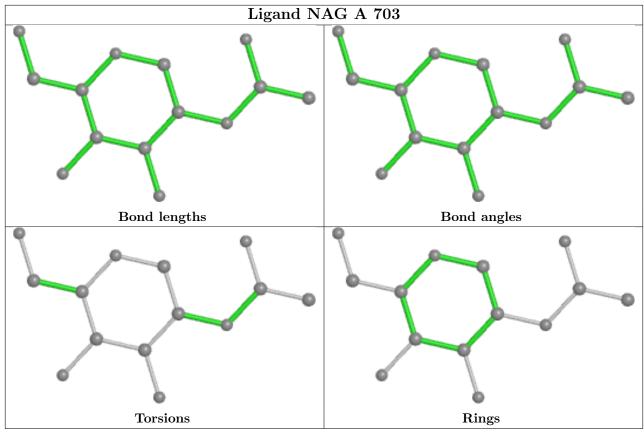
There are no ring outliers.

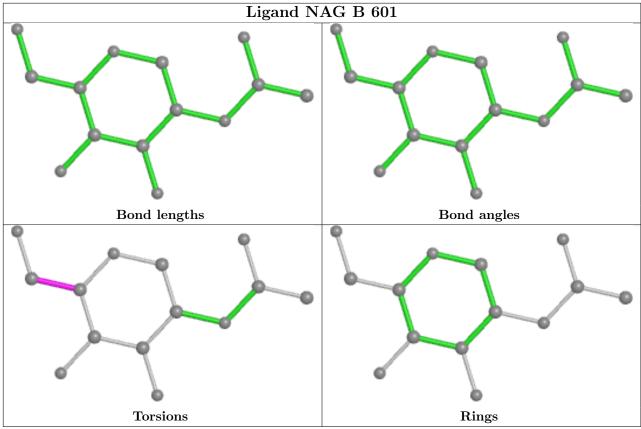
No monomer is involved in short contacts.

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 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.

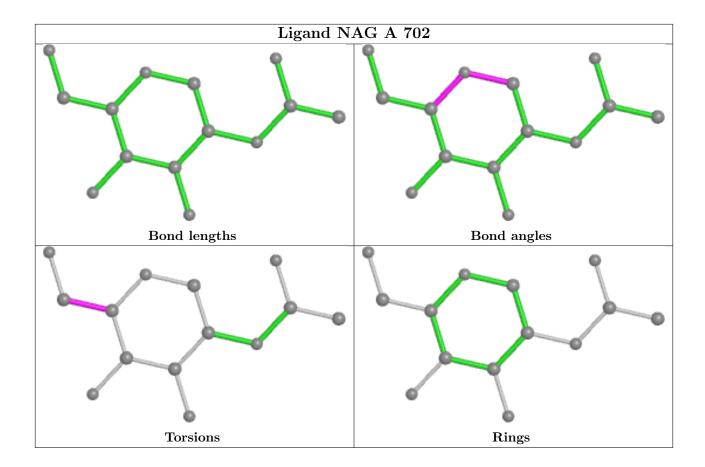












# 5.7 Other polymers (i)

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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	596/603 (98%)	0.08	31 (5%) 27 25	18, 35, 78, 148	0
2	В	195/229~(85%)	0.67	32 (16%) 1 1	28, 50, 126, 161	0
All	All	791/832 (95%)	0.23	63 (7%) 12 10	18, 39, 98, 161	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ
1	A	104	GLY	6.4
1	A	339	VAL	5.8
1	A	136	ASP	5.7
2	В	519	HIS	5.4
1	A	105	SER	5.4
2	В	385	THR	5.1
2	В	522	ALA	5.1
1	A	338	ASN	5.1
2	В	369	TYR	5.0
1	A	103	ASN	4.9
2	В	525	CYS	4.8
1	A	107	VAL	4.7
2	В	391	CYS	4.5
2	В	524	VAL	4.5
2	В	390	LEU	4.4
2	В	370	ASN	4.3
2	В	372	ALA	4.3
2	В	523	THR	4.3
2	В	517	LEU	4.2
2	В	384	PRO	4.1
2	В	386	LYS	4.1
2	В	521	PRO	4.0
2	В	518	LEU	4.0
2	В	365	TYR	4.0

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Mol	Chain	Res	Type	RSRZ	
2	В	333	THR	3.9	
2	В	527	PRO	3.8	
1	A	56	GLU	3.8	
1	A	340	GLN	3.6	
2	В	392	PHE	3.5	
2	В	526	GLY	3.4	
2	В	366	SER	3.4	
2	В	389	ASP	3.4	
2	В	387	LEU	3.3	
2	В	381	GLY	3.2	
2	В	335	LEU	3.1	
1	A	55	THR	3.0	
1	A	138	PRO	3.0	
1	A	19	SER	2.9	
1	A	341	LYS	2.9	
1	A	429	GLN	2.9	
2	В	371	SER	2.9	
1	A	20	THR	2.8	
2	В	362	VAL	2.8	
1	A	430	GLU	2.8	
1	A	139	GLN	2.7	
2	В	388	ASN	2.7	
1	A	170	SER	2.6	
1	A	57	GLU	2.4	
1	A	132	VAL	2.4	
1	A	89	GLN	2.3	
1	A	49	ASN	2.3	
1	A	58	ASN	2.3	
2	В	382	VAL	2.3	
1	A	21	ILE	2.3	
2	В	486	LEU	2.3	
1	A	60	GLN	2.2	
2	В	426	PRO	2.1	
1	A	427	ASP	2.1	
1	A	83	TYR	2.1	
1	A	87	GLU	2.1	
1	A	46	ALA	2.1	
1	A	79	LEU	2.0	
1	A	84	PRO	2.0	



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

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

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

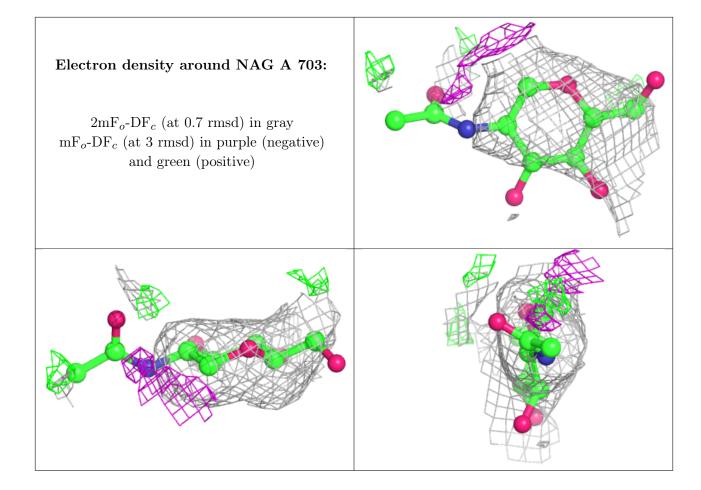
### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

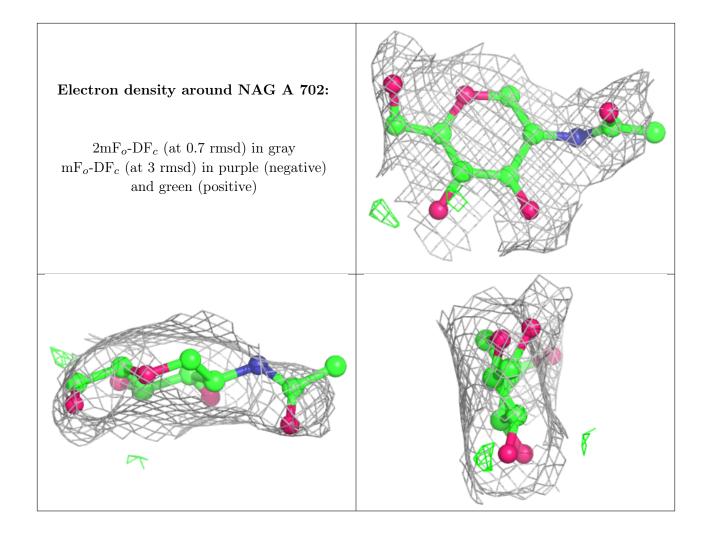
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
3	NAG	A	703	14/15	0.61	0.35	118,125,128,128	0
3	NAG	A	702	14/15	0.80	0.20	77,80,82,82	0
3	NAG	A	701	14/15	0.86	0.47	75,78,84,84	0
3	NAG	В	601	14/15	0.90	0.14	75,79,83,85	0
4	ZN	A	704	1/1	0.96	0.15	41,41,41,41	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.

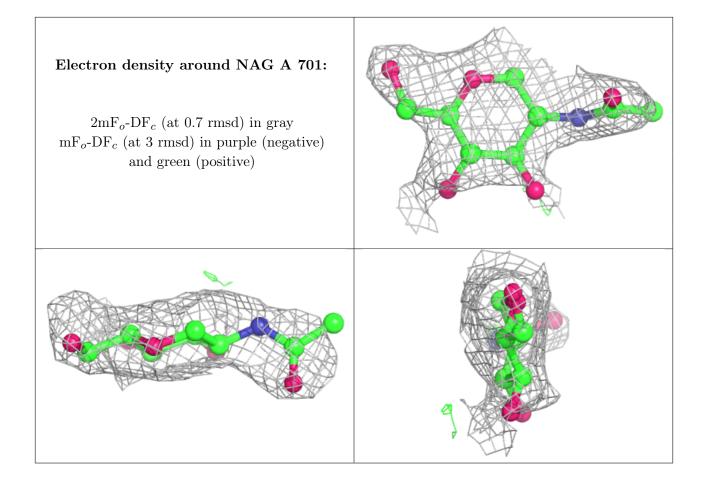




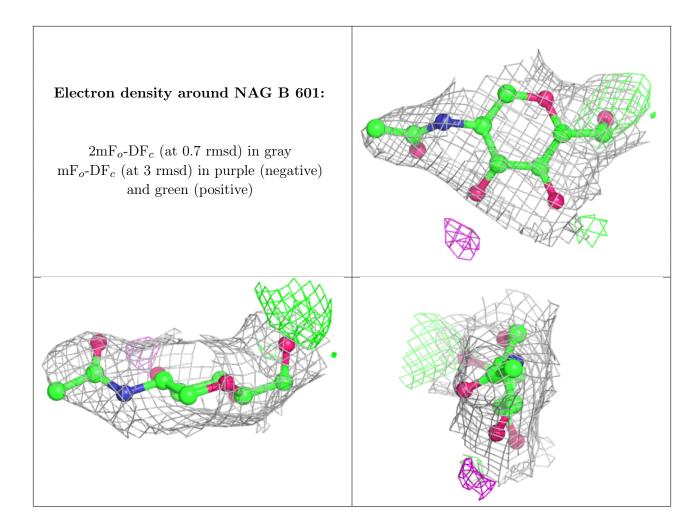












# 6.5 Other polymers (i)

There are no such residues in this entry.

