



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2025 – 08:08 PM JST

PDB ID : 8ZYF  
Title : Crystal structure of ZW2G10 Fab in complex with omicron RBD  
Authors : Yuan, H.Y.; Li, J.M.  
Deposited on : 2024-06-17  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

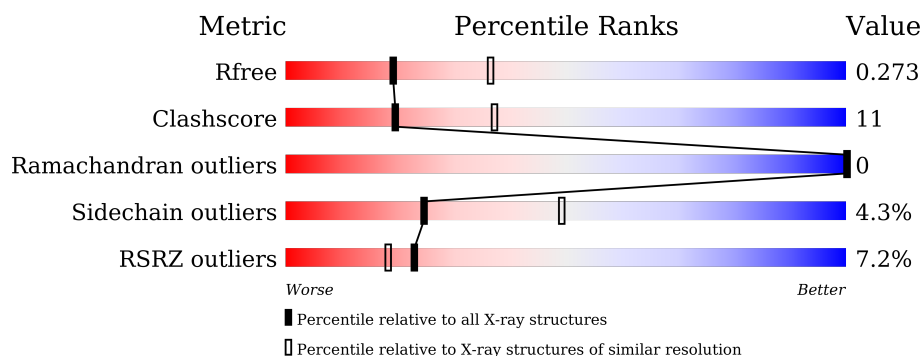
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	195	<div> <div>87%</div> <div>13%</div> </div>
1	B	195	<div> <div>4%</div> <div>85%</div> <div>14%</div> </div>
2	C	214	<div> <div>8%</div> <div>68%</div> <div>26%</div> </div>
2	D	214	<div> <div>14%</div> <div>71%</div> <div>20%</div> <div>5%</div> </div>
3	E	229	<div> <div>7%</div> <div>68%</div> <div>24%</div> <div>6%</div> </div>
3	H	229	<div> <div>5%</div> <div>62%</div> <div>16%</div> <div>22%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18204 atoms, of which 8655 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 Spike protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	H	N	O	S	0	0	0
			3053	1013	1485	265	282	8			
1	B	195	Total	C	H	N	O	S	0	0	0
			3053	1013	1485	265	282	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2

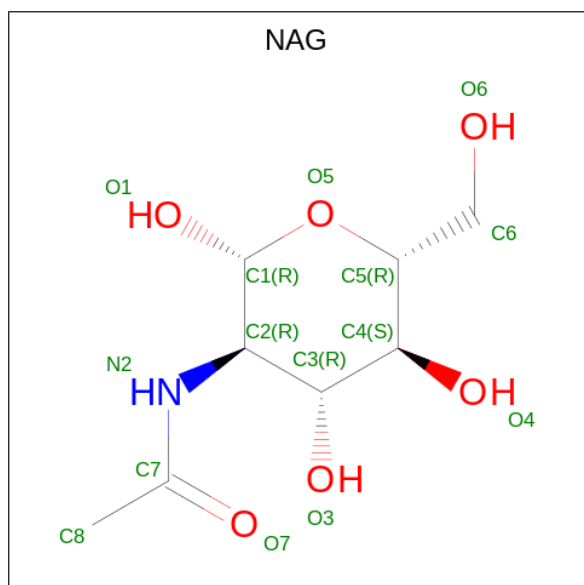
- Molecule 2 is a protein called ZW2G10 fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	203	Total	C	H	N	O	S	0	0	0
			2950	944	1438	256	308	4			
2	C	210	Total	C	H	N	O	S	0	0	0
			3047	969	1495	263	316	4			

- Molecule 3 is a protein called ZW2G10 fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	178	Total	C	H	N	O	S	0	0	0
			2655	867	1291	225	267	5			
3	E	215	Total	C	H	N	O	S	0	0	0
			3095	1033	1461	273	321	7			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

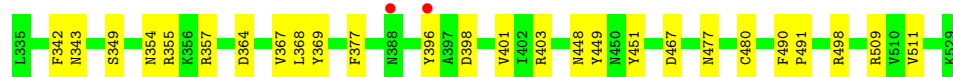
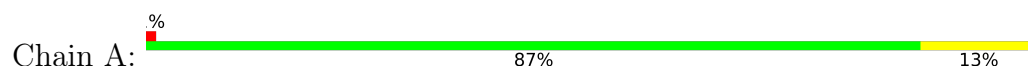
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	D	48	Total	O	0	0
			48	48		
5	H	68	Total	O	0	0
			68	68		
5	B	64	Total	O	0	0
			64	64		
5	C	38	Total	O	0	0
			38	38		
5	E	37	Total	O	0	0
			37	37		

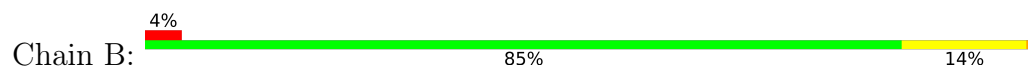
### 3 Residue-property plots [i](#)

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.

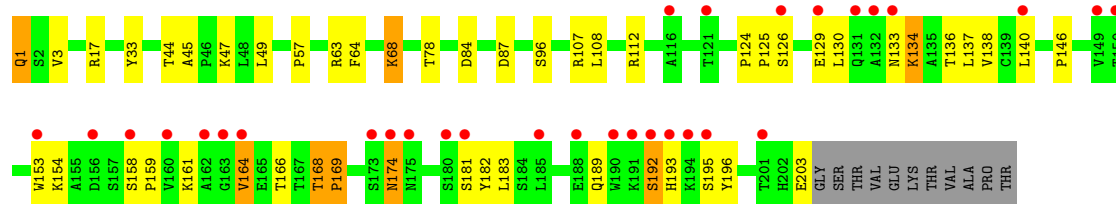
- Molecule 1: Spike protein S1



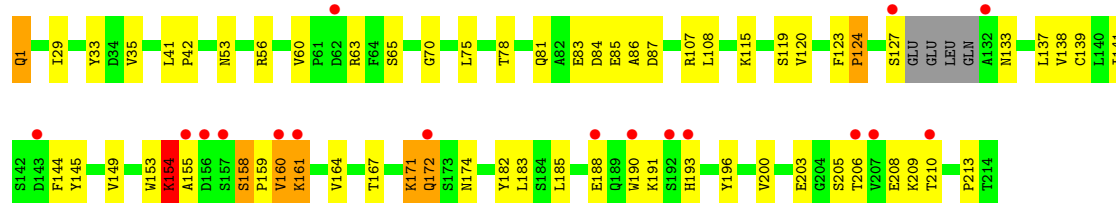
- Molecule 1: Spike protein S1



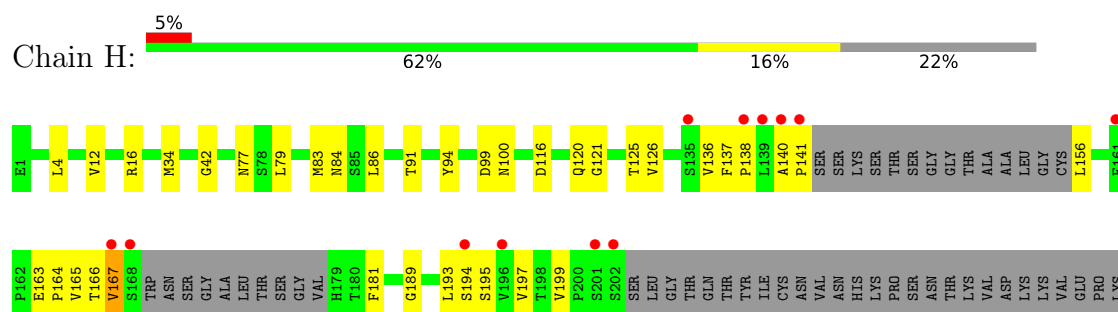
- Molecule 2: ZW2G10 fab light chain



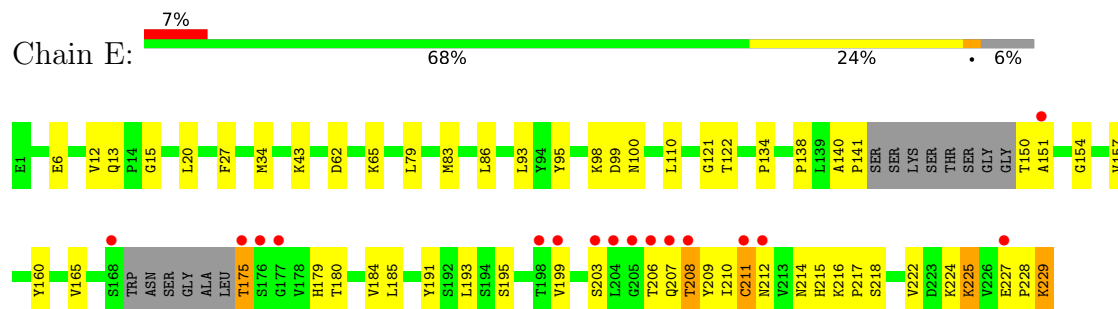
- Molecule 2: ZW2G10 fab light chain



- Molecule 3: ZW2G10 fab heavy chain



• Molecule 3: ZW2G10 fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.66Å 103.53Å 299.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.60 39.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.53-2.60) 97.9 (39.53-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.17_3644: ???)	Depositor
R, $R_{free}$	0.232 , 0.285 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	2219 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/1615	0.55	1/2196 (0.0%)
1	B	0.34	0/1615	0.51	1/2196 (0.0%)
2	C	0.69	2/1589 (0.1%)	0.86	6/2170 (0.3%)
2	D	0.60	3/1549 (0.2%)	0.72	2/2115 (0.1%)
3	E	0.45	0/1673	0.68	0/2277
3	H	0.34	0/1399	0.57	1/1905 (0.1%)
All	All	0.49	5/9440 (0.1%)	0.66	11/12859 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	169	PRO	N-CA	12.55	1.68	1.47
2	C	124	PRO	N-CA	11.94	1.67	1.47
2	D	168	THR	C-N	5.84	1.45	1.34
2	D	164	VAL	CB-CG1	-5.58	1.41	1.52
2	C	123	PHE	C-N	5.34	1.44	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	169	PRO	CA-N-CD	-8.44	99.69	111.50
1	A	477	ASN	CB-CA-C	-7.92	94.55	110.40
2	C	124	PRO	CA-N-CD	-6.50	102.40	111.50
2	D	134	LYS	N-CA-CB	-6.44	99.01	110.60
2	C	154	LYS	CB-CA-C	5.77	121.94	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	1568	1485	1507	19	0
1	B	1568	1485	1507	37	0
2	C	1552	1495	1508	52	0
2	D	1512	1438	1462	30	0
3	E	1634	1461	1582	47	0
3	H	1364	1291	1305	28	0
4	A	14	0	13	4	0
4	B	14	0	13	5	0
5	A	68	0	0	5	0
5	B	64	0	0	9	2
5	C	38	0	0	9	0
5	D	48	0	0	1	2
5	E	37	0	0	3	0
5	H	68	0	0	6	0
All	All	9549	8655	8897	205	4

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 11.

The worst 5 of 205 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:343:ASN:HD21	4:A:601:NAG:C1	1.08	1.58
1:B:343:ASN:HD21	4:B:601:NAG:C1	1.25	1.49
1:B:478:LYS:NZ	1:B:486:PHE:HD2	1.10	1.47
2:D:169:PRO:CA	2:D:169:PRO:N	1.68	1.46
2:C:124:PRO:N	2:C:124:PRO:CA	1.67	1.43

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:762:HOH:O	5:B:764:HOH:O[1_455]	1.88	0.32
5:D:310:HOH:O	5:D:339:HOH:O[4_455]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:740:HOH:O	5:B:764:HOH:O[1_455]	2.07	0.13
5:D:321:HOH:O	5:D:338:HOH:O[4_555]	2.19	0.01

## 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	193/195 (99%)	185 (96%)	8 (4%)	0	100	100
1	B	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
2	C	206/214 (96%)	189 (92%)	17 (8%)	0	100	100
2	D	201/214 (94%)	188 (94%)	13 (6%)	0	100	100
3	E	209/229 (91%)	190 (91%)	19 (9%)	0	100	100
3	H	172/229 (75%)	164 (95%)	8 (5%)	0	100	100
All	All	1174/1276 (92%)	1103 (94%)	71 (6%)	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	170/170 (100%)	169 (99%)	1 (1%)	84	94
1	B	170/170 (100%)	167 (98%)	3 (2%)	54	77
2	C	175/179 (98%)	163 (93%)	12 (7%)	13	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	170/179 (95%)	157 (92%)	13 (8%)	11	23
3	E	182/192 (95%)	169 (93%)	13 (7%)	12	26
3	H	150/192 (78%)	148 (99%)	2 (1%)	65	84
All	All	1017/1082 (94%)	973 (96%)	44 (4%)	25	49

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	174	ASN
3	E	207	GLN
2	C	188	GLU
3	E	175	THR
3	E	211	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	174	ASN
3	E	207	GLN
3	E	214	ASN
3	E	212	ASN
1	B	343	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	601	-	14,14,15	1.05	0	17,19,21	2.28	6 (35%)
4	NAG	A	601	1	14,14,15	1.24	1 (7%)	17,19,21	3.19	11 (64%)

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	B	601	-	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	-3.36	1.38	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	O5-C1-C2	-8.62	97.68	111.29
4	B	601	NAG	C1-O5-C5	5.92	120.21	112.19
4	A	601	NAG	C1-O5-C5	4.97	118.93	112.19
4	A	601	NAG	O3-C3-C2	3.64	116.99	109.47
4	A	601	NAG	C3-C4-C5	-3.42	104.13	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	5	0
4	A	601	NAG	4	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	195/195 (100%)	-0.08	2 (1%) 79 75	13, 23, 36, 52	0
1	B	195/195 (100%)	0.16	8 (4%) 42 36	15, 25, 47, 71	0
2	C	210/214 (98%)	0.64	17 (8%) 19 16	19, 34, 50, 59	0
2	D	203/214 (94%)	0.72	31 (15%) 6 5	16, 29, 62, 99	0
3	E	215/229 (93%)	0.46	16 (7%) 22 18	14, 26, 46, 65	0
3	H	178/229 (77%)	0.24	12 (6%) 25 20	13, 22, 56, 70	0
All	All	1196/1276 (93%)	0.36	86 (7%) 23 18	13, 26, 54, 99	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	160	VAL	6.8
3	E	208	THR	6.3
2	D	133	ASN	5.8
2	D	132	ALA	5.6
3	H	139	LEU	5.5

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	601	14/15	0.57	0.23	20,20,20,20	0
4	NAG	B	601	14/15	0.85	0.11	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.