

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 06:41 PM EDT

:	6PZD
:	Crystal structure of the neuraminidase stabilization mutant Y169aH from
	A/Shanghai/2/2013 (H7N9)
:	Zhu, X.; Wilson, I.A.
	2019-07-31
:	1.12 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:

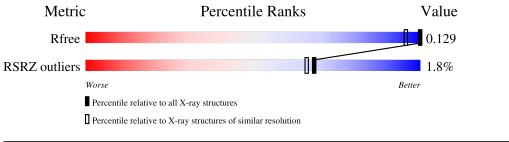
MolProbity	:	FAILED
·		1.8.5 (274361), CSD as541be (2020)
· · · · · · · · · · · · · · · · · · ·		
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.12 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1168 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



6PZD

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7369 atoms, of which 3345 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 Neuraminidase.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total 6450	C 2046	Н 3184	N 564	O 621	S 35	0	44	0

There are 6 discrepancies between the modelled and reference sequences:

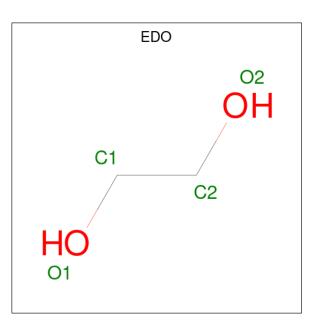
Chain	Residue	Modelled	Actual	Comment	Reference
А	77	GLY	-	expression tag	UNP V9NZ28
А	78	SER	-	expression tag	UNP V9NZ28
А	79	PRO	-	expression tag	UNP V9NZ28
А	80	SER	-	expression tag	UNP V9NZ28
А	81	ARG	-	expression tag	UNP V9NZ28
А	169A	HIS	TYR	engineered mutation	UNP V9NZ28

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyran

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	10	Total 222	$\begin{array}{c} \mathrm{C} \\ 65 \end{array}$	Н 104	N 2	O 51	0	1	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

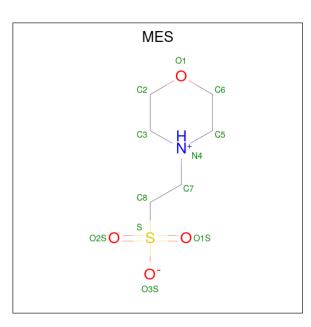




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	А	1	Total C H O	0	0	
		Ŧ	10 2 6 2	0	0	
3	А	1	Total C H O	0	0	
0	11	1	10 2 6 2	0	0	
3	٨	1	Total C H O	0	0	
5	А	1	10 2 6 2			
3	А	1	Total C H O	0	0	
5	A	1	10 2 6 2	0	0	
3	Λ	1	Total C H O	0	0	
5	3 A	1	10 2 6 2	0	0	

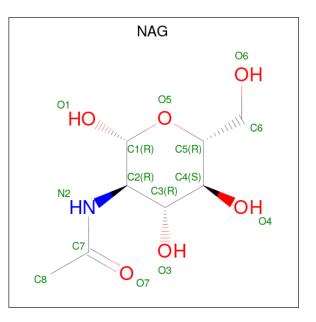
• Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	А	1	Total 25	C 6	H 13	N 1	0 4	S 1	0	0

• Molecule 5 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	
5	Δ	1	Total	С	Η	Ν	0	0	0
5	A	1	28	8	14	1	5	0	0

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Ca 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	А	593	Total 593	O 593	0	0

MolProbity failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants	182.22Å 182.22Å 182.22Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.95 - 1.12	Depositor
Resolution (A)	42.95 - 1.12	EDS
% Data completeness	99.9 (42.95-1.12)	Depositor
(in resolution range)	99.9 (42.95-1.12)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 1.12 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
D D.	0.112 , 0.128	Depositor
R, R_{free}	0.113 , 0.129	DCC
R_{free} test set	9727 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	9.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38,46.1	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms $(Å^2)$	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

11 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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	В	1	2,1	$14,\!14,\!15$	0.40	0	17,19,21	0.59	0
2	MAN	В	10	2	11,11,12	0.55	0	$15,\!15,\!17$	0.96	1 (6%)
2	NAG	В	2[A]	-	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
2	NAG	В	2[B]	-	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
2	BMA	В	3	2	11,11,12	0.86	1 (9%)	$15,\!15,\!17$	0.68	0
2	MAN	В	4	2	11,11,12	0.79	0	$15,\!15,\!17$	1.31	1 (6%)
2	MAN	В	5	2	11,11,12	0.79	0	$15,\!15,\!17$	1.00	1 (6%)
2	MAN	В	6	2	11,11,12	0.61	0	$15,\!15,\!17$	0.94	1 (6%)
2	MAN	В	7	2	11,11,12	0.81	0	$15,\!15,\!17$	0.97	1 (6%)
2	MAN	В	8	2	11,11,12	0.49	0	$15,\!15,\!17$	1.01	2 (13%)
2	MAN	В	9	2	11,11,12	0.77	0	15, 15, 17	1.02	2 (13%)

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	В	1	2,1	-	0/6/23/26	0/1/1/1
2	MAN	В	10	2	-	0/2/19/22	0/1/1/1
2	NAG	В	2[A]	-	-	0/6/23/26	0/1/1/1
2	NAG	В	2[B]	-	-	0/6/23/26	0/1/1/1
2	BMA	В	3	2	-	0/2/19/22	0/1/1/1
2	MAN	В	4	2	-	0/2/19/22	0/1/1/1
2	MAN	В	5	2	-	0/2/19/22	0/1/1/1
2	MAN	В	6	2	-	0/2/19/22	0/1/1/1
2	MAN	В	7	2	-	0/2/19/22	0/1/1/1
2	MAN	В	8	2	-	0/2/19/22	0/1/1/1
2	MAN	В	9	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	3	BMA	O5-C1	-2.23	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	4	MAN	O2-C2-C1	-3.53	101.93	109.15
2	В	5	MAN	C1-O5-C5	3.38	116.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	9	MAN	C1-O5-C5	2.61	115.72	112.19
2	В	8	MAN	C1-O5-C5	2.49	115.57	112.19
2	В	6	MAN	C1-O5-C5	2.48	115.56	112.19
2	В	10	MAN	C1-O5-C5	2.40	115.44	112.19
2	В	9	MAN	O2-C2-C3	-2.29	105.55	110.14
2	В	8	MAN	O2-C2-C3	-2.25	105.63	110.14
2	В	7	MAN	C1-O5-C5	2.19	115.16	112.19
2	В	2[A]	NAG	O3-C3-C2	2.02	113.64	109.47
2	В	2[B]	NAG	O3-C3-C2	2.02	113.64	109.47

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There are no chirality outliers.

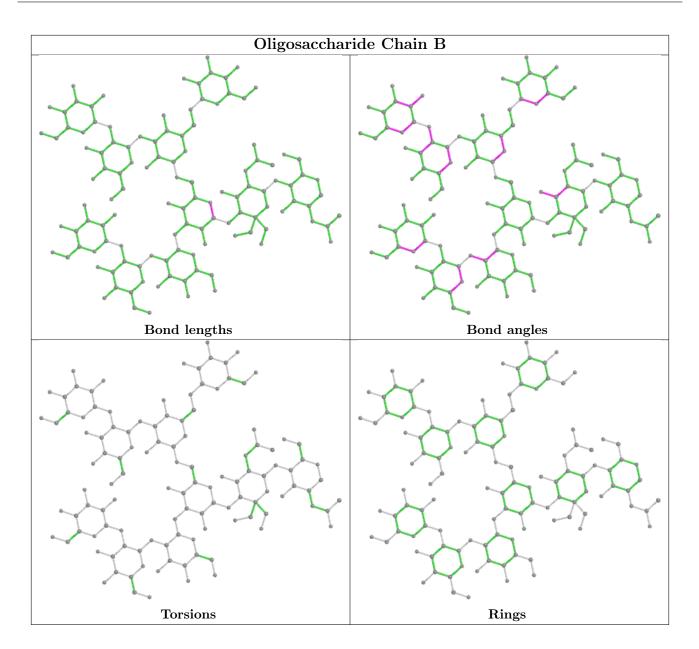
There are no torsion outliers.

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.





4.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	Res	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
IVIOI	Type		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	EDO	А	514	-	$3,\!3,\!3$	0.34	0	$2,\!2,\!2$	0.24	0



Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
10101	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	EDO	А	512	-	$3,\!3,\!3$	0.59	0	2,2,2	0.35	0
3	EDO	А	511	-	$3,\!3,\!3$	0.51	0	2,2,2	0.27	0
4	MES	А	516	-	12,12,12	1.73	1 (8%)	14,16,16	1.16	1 (7%)
5	NAG	А	517	1	14,14,15	0.55	0	17,19,21	0.46	0
3	EDO	А	515	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	А	513	-	3,3,3	0.52	0	2,2,2	0.40	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
3	EDO	А	514	-	-	0/1/1/1	-
3	EDO	А	512	-	-	0/1/1/1	-
3	EDO	А	511	-	-	0/1/1/1	-
4	MES	А	516	-	-	0/6/14/14	0/1/1/1
5	NAG	А	517	1	-	0/6/23/26	0/1/1/1
3	EDO	А	515	-	-	0/1/1/1	-
3	EDO	А	513	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	516	MES	C8-S	-5.62	1.69	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	516	MES	O1S-S-C8	3.12	110.68	106.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	513	EDO	O1-C1-C2-O2

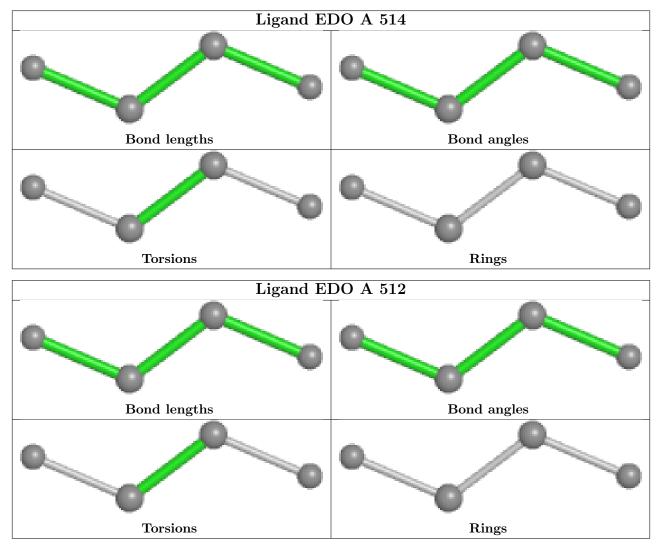
There are no ring outliers.

No monomer is involved in short contacts.

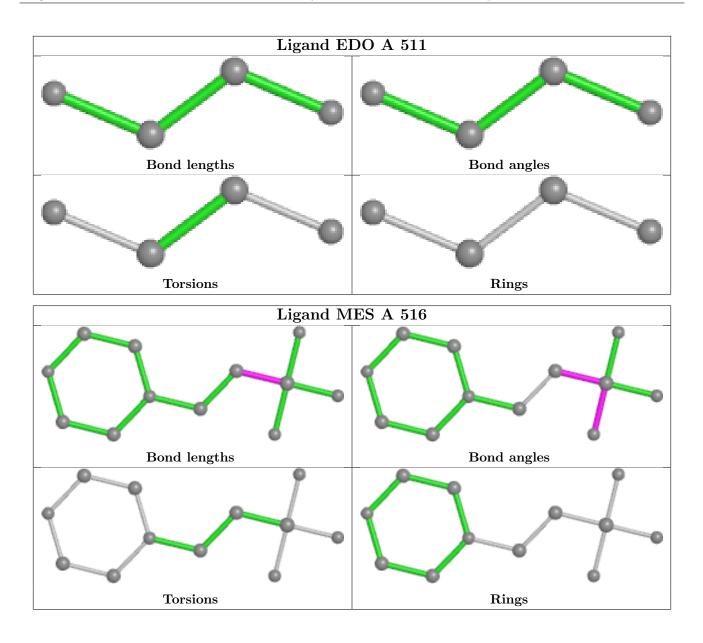
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



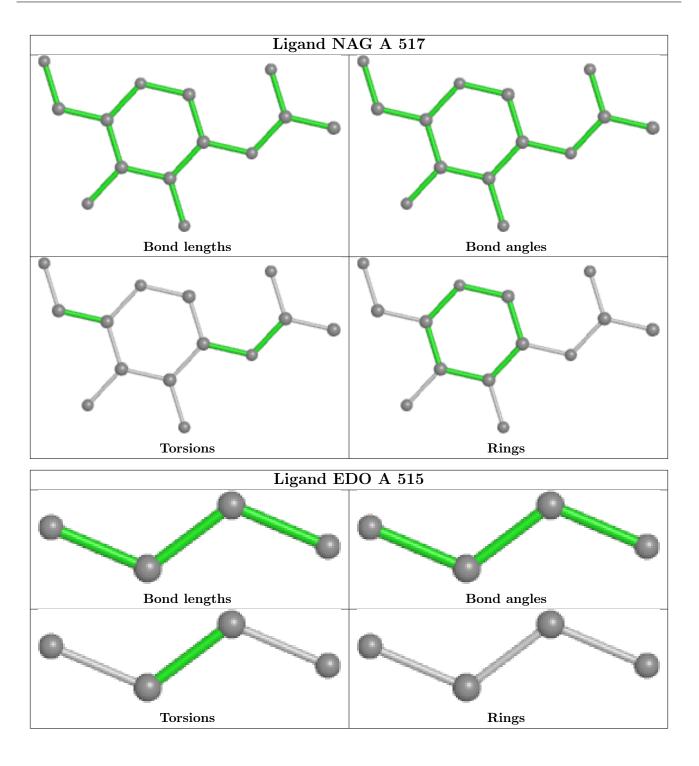
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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.



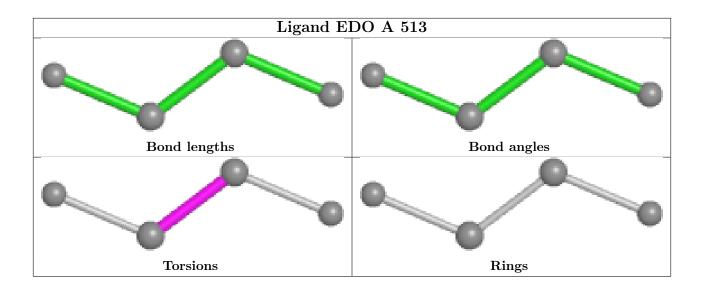












4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 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	389/393~(98%)	-0.20	7 (1%)	68	66	6, 9, 15, 53	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	81	ARG	9.4	
1	А	468	LEU	3.9	
1	А	150[A]	HIS	2.5	
1	А	463[A]	LYS	2.4	
1	А	83	ASN	2.2	
1	А	435	LYS	2.1	
1	А	465[A]	GLU	2.0	

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

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

5.3 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	MAN	В	10	11/12	0.69	0.26	$30,\!48,\!56,\!61$	0
2	MAN	В	9	11/12	0.87	0.23	$19,\!33,\!51,\!52$	0
2	MAN	В	7	11/12	0.91	0.11	14,19,25,25	0
2	MAN	В	8	11/12	0.91	0.16	19,26,38,38	0
2	MAN	В	5	11/12	0.96	0.11	11,15,18,21	0

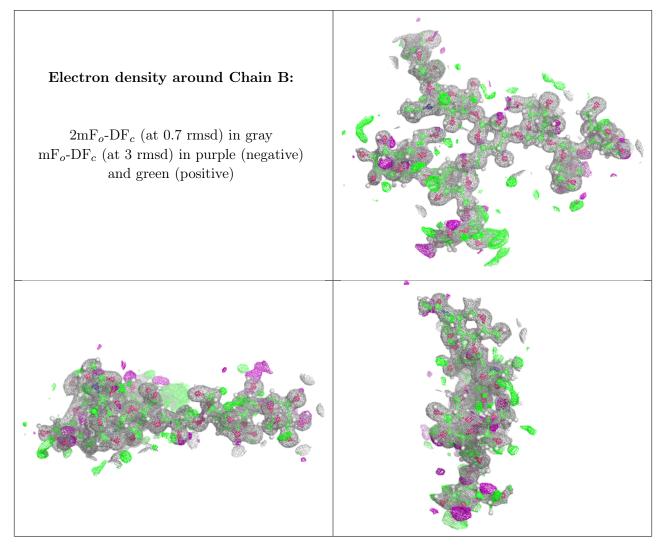
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	BMA	В	3	11/12	0.97	0.08	$10,\!13,\!15,\!18$	0
2	MAN	В	4	11/12	0.97	0.09	11,13,22,23	0
2	NAG	В	1	14/15	0.97	0.09	$10,\!12,\!25,\!25$	0
2	MAN	В	6	11/12	0.97	0.11	$11,\!13,\!15,\!16$	0
2	NAG	В	2[A]	14/15	0.98	0.08	10,12,18,20	5
2	NAG	В	2[B]	14/15	0.98	0.08	10,12,17,23	5

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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.



5.4 Ligands (i)

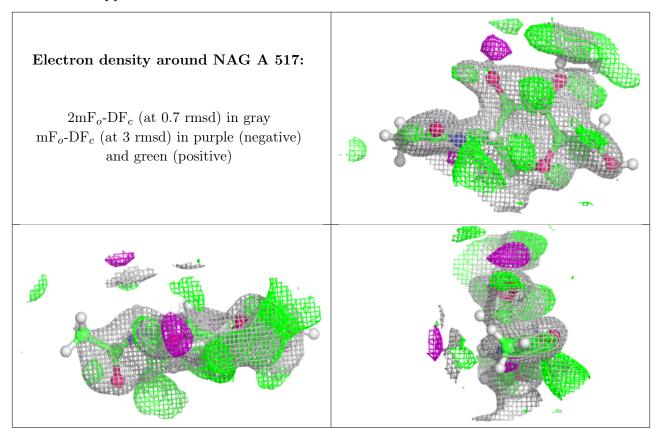
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column



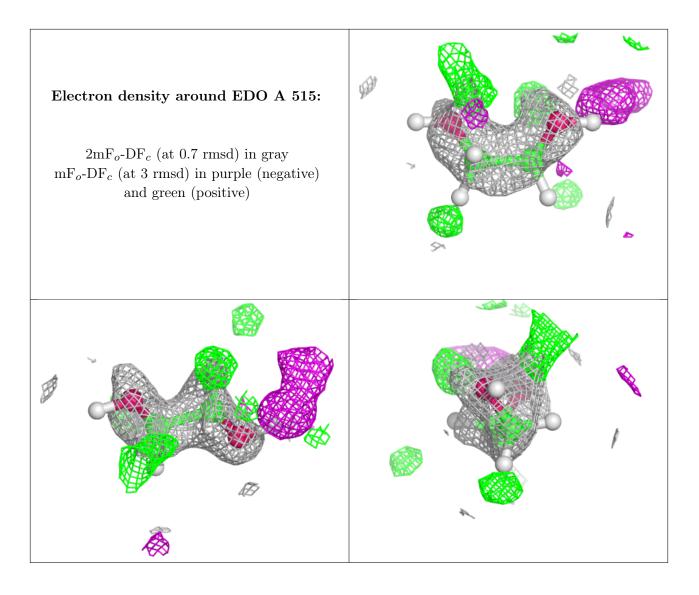
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
5	NAG	А	517	14/15	0.80	0.18	24,42,52,61	0
3	EDO	А	515	4/4	0.82	0.12	40,48,50,54	0
3	EDO	А	513	4/4	0.86	0.15	$20,\!48,\!59,\!65$	0
3	EDO	А	511	4/4	0.90	0.24	16,23,36,43	0
4	MES	А	516	12/12	0.91	0.11	12,16,23,29	0
3	EDO	А	512	4/4	0.92	0.14	17,20,24,24	0
3	EDO	А	514	4/4	0.93	0.11	17,22,25,27	0
6	CA	А	518	1/1	1.00	0.07	9,9,9,9	1

labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

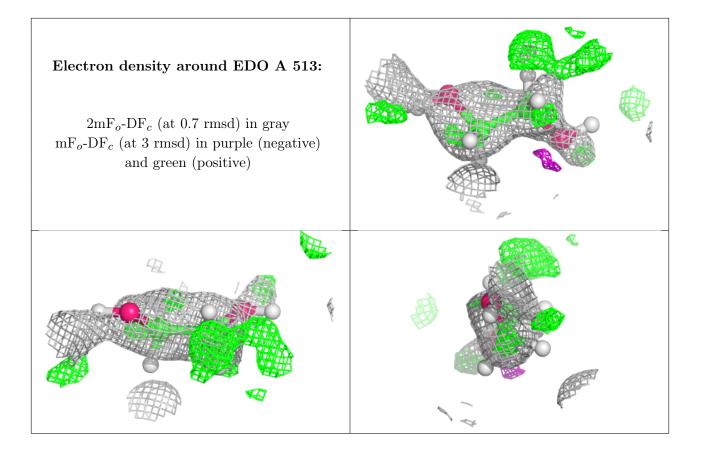
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



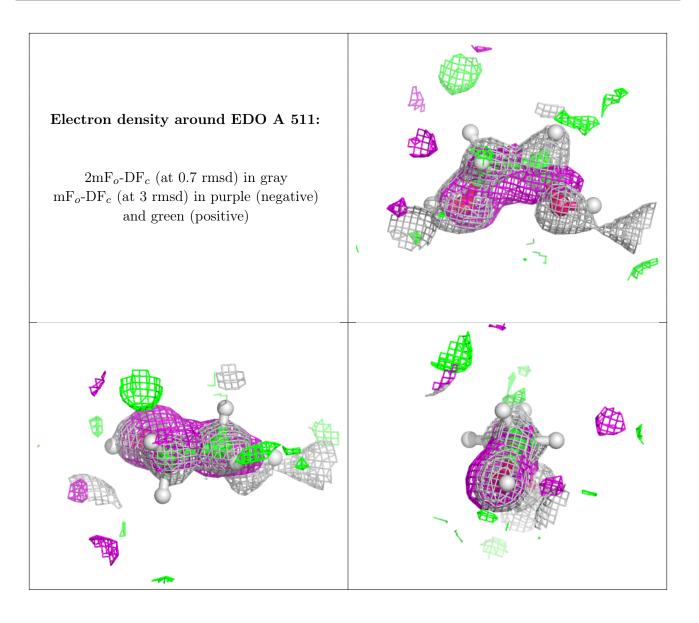




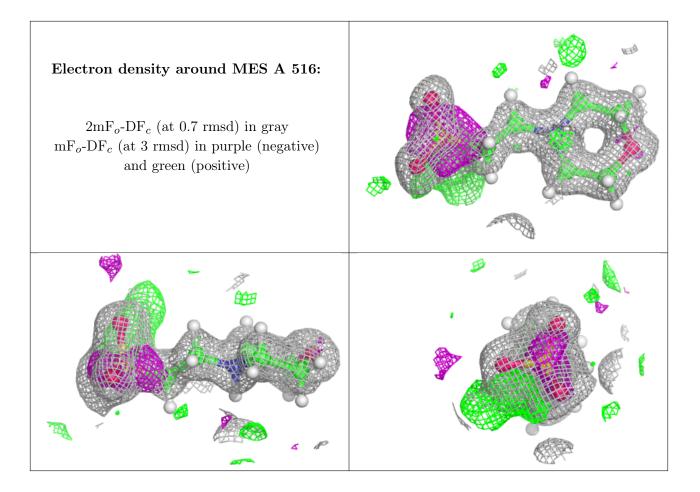




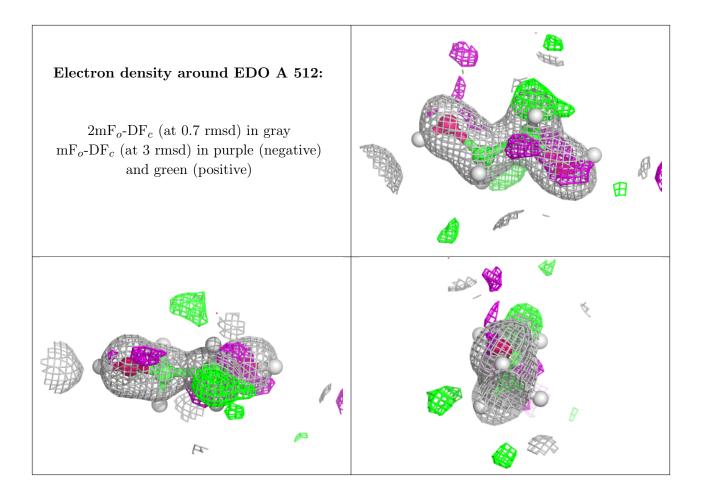




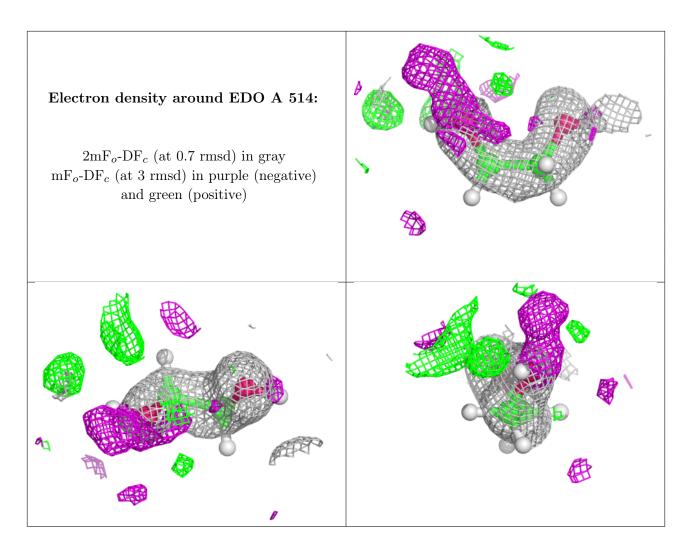




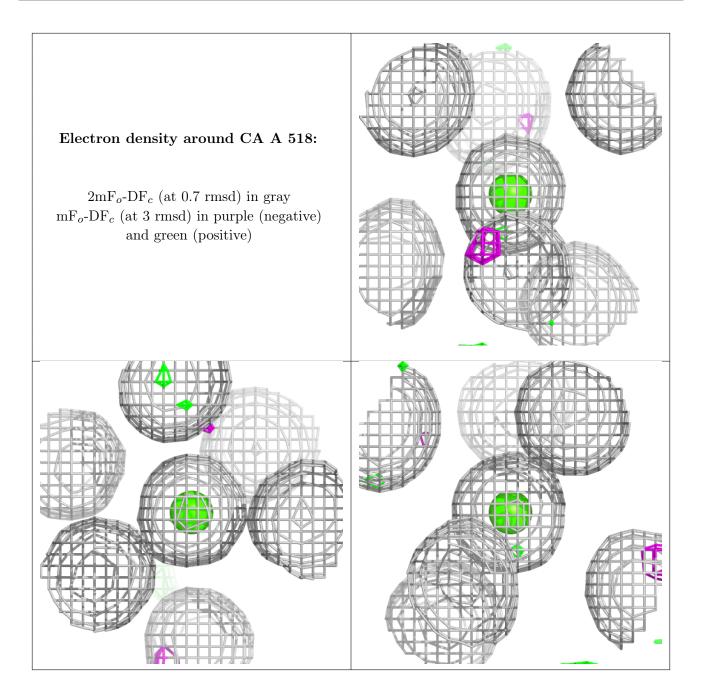












5.5 Other polymers (i)

There are no such residues in this entry.

