



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 04:40 AM EDT

PDB ID : 3C6E
Title : Crystal structure of the precursor membrane protein- envelope protein heterodimer from the dengue 2 virus at neutral pH
Authors : Li, L.
Deposited on : 2008-02-04
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

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>.

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) : 1.13
EDS : 2.35
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

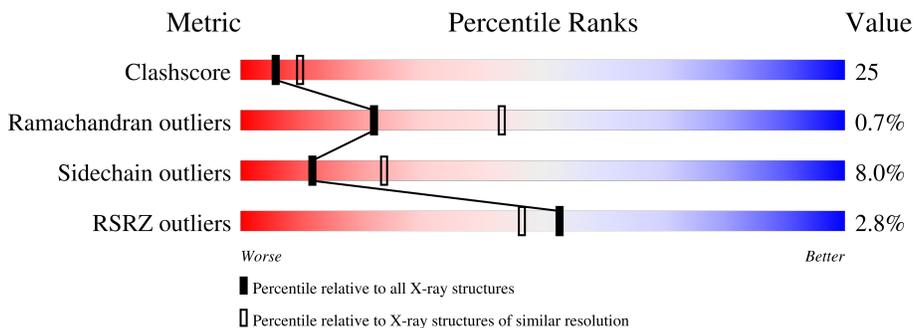
1 Overall quality at a glance

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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 ≥ 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	402	
2	C	130	
3	B	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	1	X	-	X	-
3	MAN	B	3	-	-	-	X
3	MAN	B	4	X	-	-	X
4	NDG	C	1396	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3811 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3046	1926	524	569	27	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O09234
A	-6	GLU	-	expression tag	UNP O09234
A	-5	ASN	-	expression tag	UNP O09234
A	-4	LEU	-	expression tag	UNP O09234
A	-3	TYR	-	expression tag	UNP O09234
A	-2	PHE	-	expression tag	UNP O09234
A	-1	GLN	-	expression tag	UNP O09234
A	0	GLY	-	expression tag	UNP O09234

- Molecule 2 is a protein called prM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	81	640	396	106	128	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

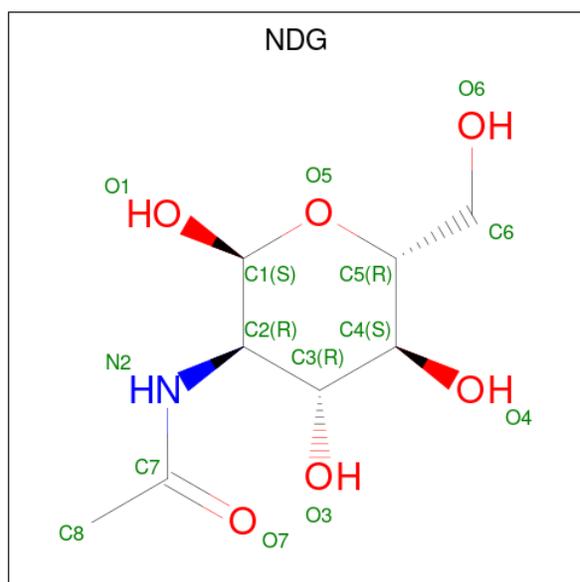
Chain	Residue	Modelled	Actual	Comment	Reference
C	87	SER	ARG	engineered mutation	UNP O09234
C	88	THR	ARG	engineered mutation	UNP O09234
C	91	SER	ARG	engineered mutation	UNP O09234

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



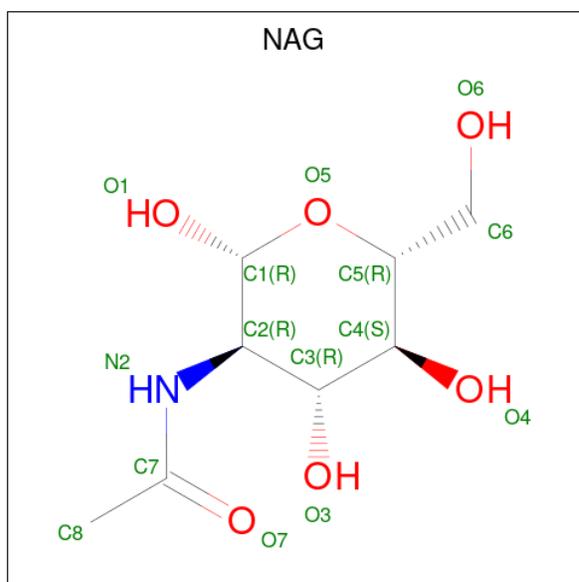
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
3	B	4	50	28	2	20	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	C	1	15	8	1	6	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	15	8	1	6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	38	38	38	0	0
6	C	7	7	7	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.10Å 108.37Å 108.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 43.24 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.5 (43.24-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.293 0.250 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.019 for -h,l,k	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3811	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: NDG, NAG, MAN

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	0.54	2/3106 (0.1%)	0.78	7/4186 (0.2%)
2	C	0.61	2/652 (0.3%)	0.69	1/883 (0.1%)
All	All	0.55	4/3758 (0.1%)	0.77	8/5069 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	C-N	-15.23	1.05	1.34
1	A	334	LYS	C-N	-13.74	1.02	1.34
2	C	48	THR	C-N	-9.51	1.12	1.34
2	C	49	ILE	C-N	-7.05	1.17	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	LYS	O-C-N	-9.85	106.94	122.70
1	A	384	PRO	N-CA-C	-8.39	90.28	112.10
1	A	383	GLU	N-CA-C	8.19	133.10	111.00
1	A	332	PRO	N-CA-C	-8.06	91.14	112.10
1	A	334	LYS	C-N-CA	7.27	139.88	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	49	ILE	Mainchain

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	3046	0	3045	151	0
2	C	640	0	609	30	0
3	B	50	0	39	12	0
4	C	15	0	12	10	0
5	C	15	0	15	6	0
6	A	38	0	0	4	0
6	C	7	0	0	0	0
All	All	3811	0	3720	188	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 25.

The worst 5 of 188 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:188:ARG:HD3	1:A:284:LYS:HD2	1.24	1.11
2:C:2:HIS:NE2	3:B:4:MAN:O2	1.96	0.98
1:A:198:LEU:HD22	1:A:277:LEU:HD13	1.46	0.97
2:C:2:HIS:HE2	3:B:4:MAN:HO2	1.13	0.93
1:A:75:PRO:O	1:A:76:THR:HB	1.72	0.87

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	380/402 (94%)	345 (91%)	32 (8%)	3 (1%)	19	39
2	C	79/130 (61%)	70 (89%)	9 (11%)	0	100	100
All	All	459/532 (86%)	415 (90%)	41 (9%)	3 (1%)	22	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	383	GLU
1	A	384	PRO

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	339/348 (97%)	316 (93%)	23 (7%)	16	32
2	C	75/118 (64%)	65 (87%)	10 (13%)	4	7
All	All	414/466 (89%)	381 (92%)	33 (8%)	12	24

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	41	LEU
2	C	48	THR
2	C	71	THR
1	A	323	ARG
1	A	300	SER

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

Mol	Chain	Res	Type
1	A	261	HIS
1	A	316	GLN
2	C	17	GLN
2	C	7	ASN
1	A	200	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](#)

4 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	B	1	1,3	14,14,15	0.52	0	17,19,21	4.72	2 (11%)
3	NDG	B	2	3	14,14,15	1.86	1 (7%)	17,19,21	1.69	4 (23%)
3	MAN	B	3	3	11,11,12	0.87	1 (9%)	15,15,17	0.89	1 (6%)
3	MAN	B	4	3	11,11,12	1.10	1 (9%)	15,15,17	2.91	4 (26%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	1,3	1/1/5/7	5/6/23/26	0/1/1/1
3	NDG	B	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	3	3	-	2/2/19/22	0/1/1/1
3	MAN	B	4	3	1/1/4/5	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	NDG	C2-N2	-6.53	1.35	1.46
3	B	4	MAN	C6-C5	-2.49	1.43	1.51
3	B	3	MAN	O3-C3	2.28	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O4-C4-C5	17.43	152.57	109.30
3	B	4	MAN	C6-C5-C4	8.46	132.82	113.00
3	B	1	NAG	O4-C4-C3	-8.31	91.13	110.35
3	B	4	MAN	O5-C5-C6	5.42	115.70	107.20
3	B	2	NDG	C2-N2-C7	4.64	129.51	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1	NAG	C1
3	B	4	MAN	C5

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NDG	C8-C7-N2-C2
3	B	2	NDG	O7-C7-N2-C2
3	B	4	MAN	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 12 short contacts:

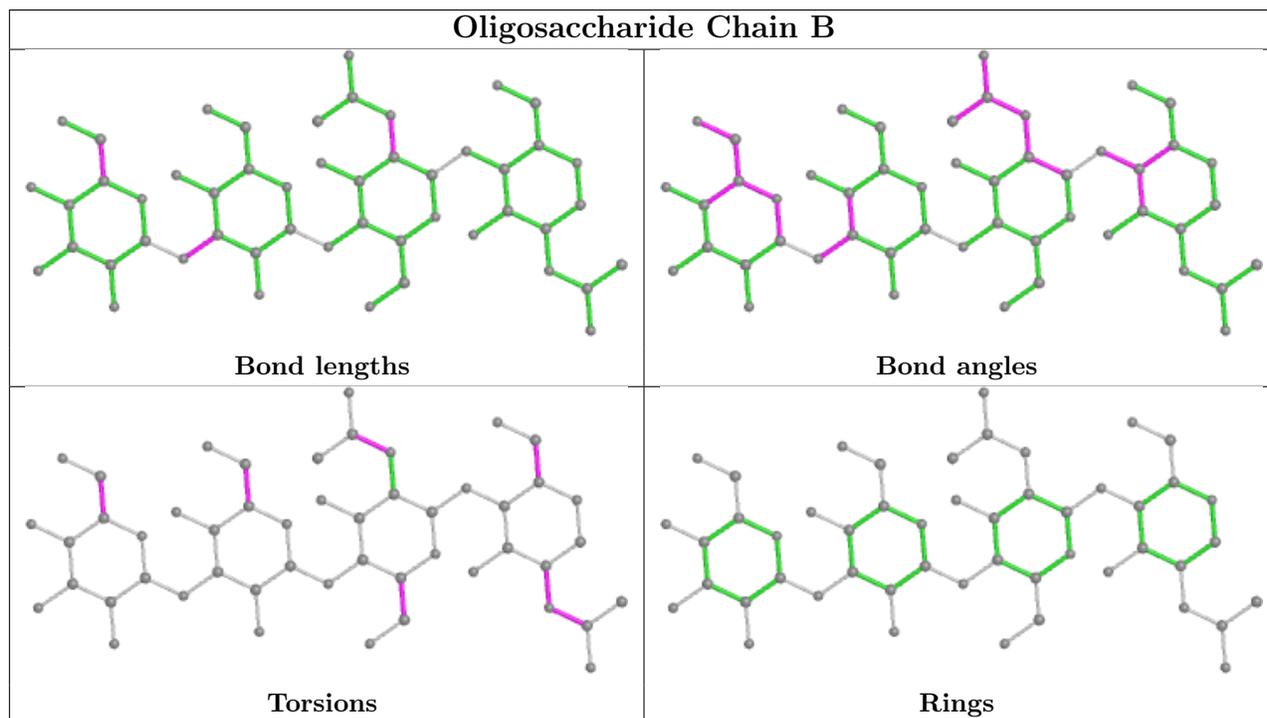
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	NDG	4	0
3	B	1	NAG	7	0
3	B	4	MAN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3	MAN	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 oligosaccharide.



5.6 Ligand geometry [i](#)

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	NDG	C	1396	-	15,15,15	0.41	0	21,21,21	0.77	0
5	NAG	C	1397	-	15,15,15	0.46	0	21,21,21	0.63	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	NDG	C	1396	-	-	3/6/26/26	0/1/1/1
5	NAG	C	1397	-	-	5/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1396	NDG	C1-C2-N2-C7
5	C	1397	NAG	C1-C2-N2-C7
5	C	1397	NAG	C8-C7-N2-C2
5	C	1397	NAG	O7-C7-N2-C2
4	C	1396	NDG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1396	NDG	10	0
5	C	1397	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	49:ILE	C	50:THR	N	1.17
1	C	48:THR	C	49:ILE	N	1.12
1	A	335:ILE	C	336:PRO	N	1.05
1	A	334:LYS	C	335:ILE	N	1.02

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, 95th 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	390/402 (97%)	0.21	13 (3%) 46 39	27, 62, 105, 141	0
2	C	81/130 (62%)	-0.02	0 100 100	23, 51, 79, 95	0
All	All	471/532 (88%)	0.17	13 (2%) 53 46	23, 59, 104, 141	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	ASP	4.0
1	A	329	ASP	3.7
1	A	149	HIS	2.8
1	A	203	ASN	2.8
1	A	56	LEU	2.5

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

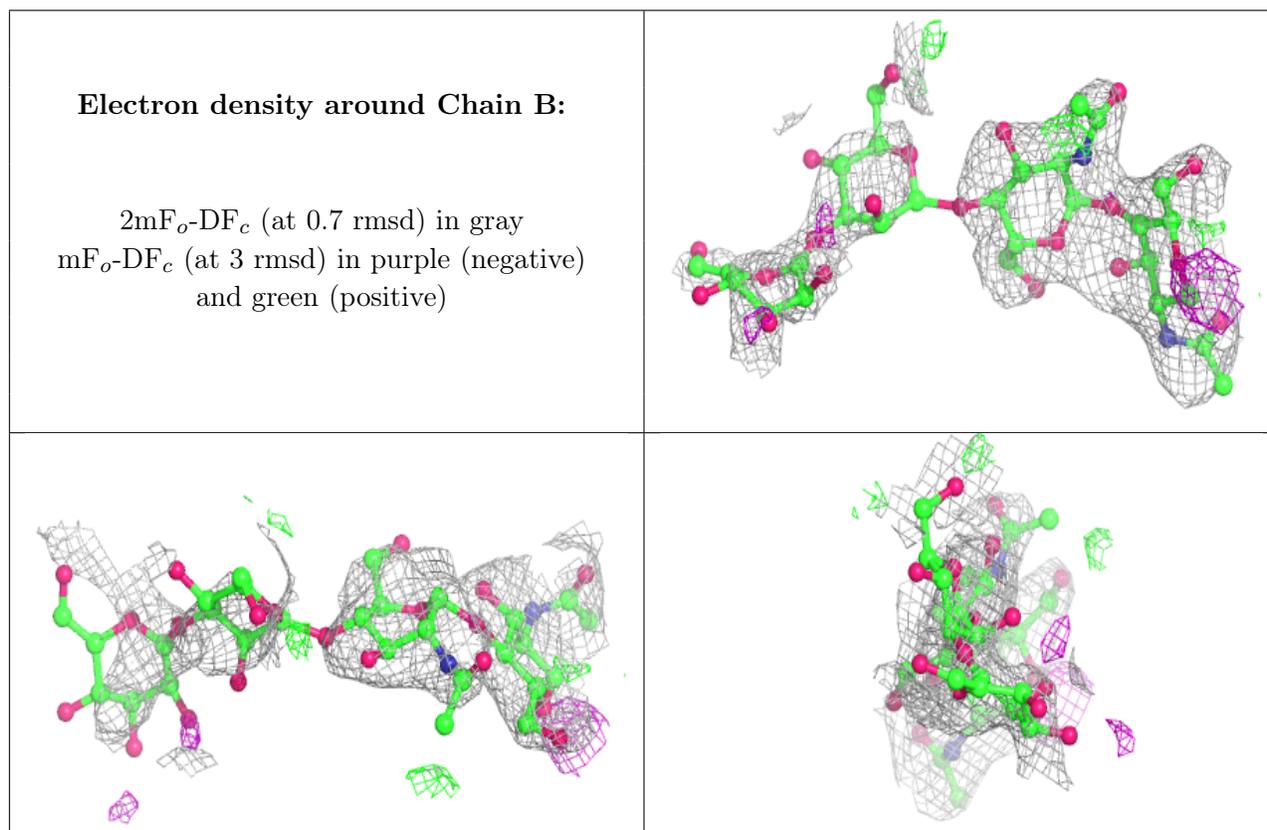
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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, 95th 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	MAN	B	3	11/12	0.46	0.54	169,184,191,193	0
3	MAN	B	4	11/12	0.56	0.53	171,172,175,177	0
3	NAG	B	1	14/15	0.80	0.21	88,89,90,90	0
3	NDG	B	2	14/15	0.83	0.29	103,107,120,144	0

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, 95th 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(\AA^2)	Q<0.9
5	NAG	C	1397	15/15	0.73	0.24	88,90,92,93	0
4	NDG	C	1396	15/15	0.89	0.18	58,63,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.