



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 05:08 pm GMT

PDB ID : 2B9B
Title : Structure of the Parainfluenza Virus 5 F Protein in its Metastable, Pre-fusion Conformation
Authors : Yin, H.-S.; Wen, X.; Paterson, R.G.; Lamb, R.A.; Jardetzky, T.S.
Deposited on : 2005-10-11
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

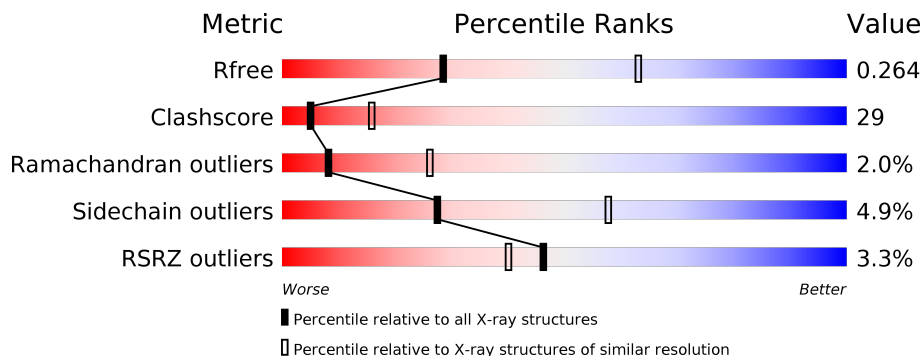
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	111664	2715 (2.90-2.82)
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	497	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>• •</div> </div> </div>
1	B	497	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>40%</div> <div>• •</div> </div> </div>
1	C	497	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>• •</div> </div> </div>

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
2	NAG	C	1065	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10922 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3538	2241	589	687	21			
1	B	482	Total	C	N	O	S	0	0	0
			3547	2245	588	693	21			
1	C	481	Total	C	N	O	S	0	0	0
			3539	2240	586	692	21			

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	DELETION	UNP P04849
A	?	-	ARG	DELETION	UNP P04849
A	478	GLU	-	CLONING ARTIFACT	UNP P04849
A	479	ASP	-	CLONING ARTIFACT	UNP P04849
A	480	LYS	-	CLONING ARTIFACT	UNP P04849
A	481	ILE	-	CLONING ARTIFACT	UNP P04849
A	482	GLU	-	CLONING ARTIFACT	UNP P04849
A	483	GLU	-	CLONING ARTIFACT	UNP P04849
A	484	ILE	-	CLONING ARTIFACT	UNP P04849
A	485	LEU	-	CLONING ARTIFACT	UNP P04849
A	486	SER	-	CLONING ARTIFACT	UNP P04849
A	487	LYS	-	CLONING ARTIFACT	UNP P04849
A	488	ILE	-	CLONING ARTIFACT	UNP P04849
A	489	TYR	-	CLONING ARTIFACT	UNP P04849
A	490	HIS	-	CLONING ARTIFACT	UNP P04849
A	491	ILE	-	CLONING ARTIFACT	UNP P04849
A	492	GLU	-	CLONING ARTIFACT	UNP P04849
A	493	ASN	-	CLONING ARTIFACT	UNP P04849
A	492	GLU	-	CLONING ARTIFACT	UNP P04849
A	495	ILE	-	CLONING ARTIFACT	UNP P04849
A	496	ALA	-	CLONING ARTIFACT	UNP P04849
A	497	ARG	-	CLONING ARTIFACT	UNP P04849
A	498	ILE	-	CLONING ARTIFACT	UNP P04849

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Chain	Residue	Modelled	Actual	Comment	Reference
A	499	LYS	-	CLONING ARTIFACT	UNP P04849
A	500	LYS	-	CLONING ARTIFACT	UNP P04849
A	501	LEU	-	CLONING ARTIFACT	UNP P04849
A	502	ILE	-	CLONING ARTIFACT	UNP P04849
A	503	GLY	-	CLONING ARTIFACT	UNP P04849
A	504	GLU	-	CLONING ARTIFACT	UNP P04849
A	505	ALA	-	CLONING ARTIFACT	UNP P04849
A	506	PRO	-	CLONING ARTIFACT	UNP P04849
A	507	GLY	-	CLONING ARTIFACT	UNP P04849
A	508	GLY	-	CLONING ARTIFACT	UNP P04849
A	509	ILE	-	CLONING ARTIFACT	UNP P04849
A	510	GLU	-	CLONING ARTIFACT	UNP P04849
A	511	GLY	-	CLONING ARTIFACT	UNP P04849
A	512	ARG	-	CLONING ARTIFACT	UNP P04849
A	513	HIS	-	EXPRESSION TAG	UNP P04849
A	514	HIS	-	EXPRESSION TAG	UNP P04849
A	513	HIS	-	EXPRESSION TAG	UNP P04849
A	514	HIS	-	EXPRESSION TAG	UNP P04849
A	515	HIS	-	EXPRESSION TAG	UNP P04849
A	516	HIS	-	EXPRESSION TAG	UNP P04849
B	?	-	ARG	DELETION	UNP P04849
B	?	-	ARG	DELETION	UNP P04849
B	478	GLU	-	CLONING ARTIFACT	UNP P04849
B	479	ASP	-	CLONING ARTIFACT	UNP P04849
B	480	LYS	-	CLONING ARTIFACT	UNP P04849
B	481	ILE	-	CLONING ARTIFACT	UNP P04849
B	482	GLU	-	CLONING ARTIFACT	UNP P04849
B	483	GLU	-	CLONING ARTIFACT	UNP P04849
B	484	ILE	-	CLONING ARTIFACT	UNP P04849
B	485	LEU	-	CLONING ARTIFACT	UNP P04849
B	486	SER	-	CLONING ARTIFACT	UNP P04849
B	487	LYS	-	CLONING ARTIFACT	UNP P04849
B	488	ILE	-	CLONING ARTIFACT	UNP P04849
B	489	TYR	-	CLONING ARTIFACT	UNP P04849
B	490	HIS	-	CLONING ARTIFACT	UNP P04849
B	491	ILE	-	CLONING ARTIFACT	UNP P04849
B	492	GLU	-	CLONING ARTIFACT	UNP P04849
B	493	ASN	-	CLONING ARTIFACT	UNP P04849
B	492	GLU	-	CLONING ARTIFACT	UNP P04849
B	495	ILE	-	CLONING ARTIFACT	UNP P04849
B	496	ALA	-	CLONING ARTIFACT	UNP P04849
B	497	ARG	-	CLONING ARTIFACT	UNP P04849

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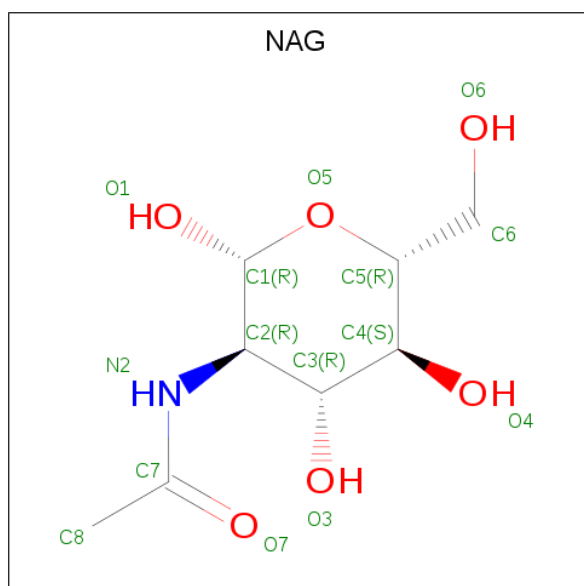
Chain	Residue	Modelled	Actual	Comment	Reference
B	498	ILE	-	CLONING ARTIFACT	UNP P04849
B	499	LYS	-	CLONING ARTIFACT	UNP P04849
B	500	LYS	-	CLONING ARTIFACT	UNP P04849
B	501	LEU	-	CLONING ARTIFACT	UNP P04849
B	502	ILE	-	CLONING ARTIFACT	UNP P04849
B	503	GLY	-	CLONING ARTIFACT	UNP P04849
B	504	GLU	-	CLONING ARTIFACT	UNP P04849
B	505	ALA	-	CLONING ARTIFACT	UNP P04849
B	506	PRO	-	CLONING ARTIFACT	UNP P04849
B	507	GLY	-	CLONING ARTIFACT	UNP P04849
B	508	GLY	-	CLONING ARTIFACT	UNP P04849
B	509	ILE	-	CLONING ARTIFACT	UNP P04849
B	510	GLU	-	CLONING ARTIFACT	UNP P04849
B	511	GLY	-	CLONING ARTIFACT	UNP P04849
B	512	ARG	-	CLONING ARTIFACT	UNP P04849
B	513	HIS	-	EXPRESSION TAG	UNP P04849
B	514	HIS	-	EXPRESSION TAG	UNP P04849
B	513	HIS	-	EXPRESSION TAG	UNP P04849
B	514	HIS	-	EXPRESSION TAG	UNP P04849
B	515	HIS	-	EXPRESSION TAG	UNP P04849
B	516	HIS	-	EXPRESSION TAG	UNP P04849
C	?	-	ARG	DELETION	UNP P04849
C	?	-	ARG	DELETION	UNP P04849
C	478	GLU	-	CLONING ARTIFACT	UNP P04849
C	479	ASP	-	CLONING ARTIFACT	UNP P04849
C	480	LYS	-	CLONING ARTIFACT	UNP P04849
C	481	ILE	-	CLONING ARTIFACT	UNP P04849
C	482	GLU	-	CLONING ARTIFACT	UNP P04849
C	483	GLU	-	CLONING ARTIFACT	UNP P04849
C	484	ILE	-	CLONING ARTIFACT	UNP P04849
C	485	LEU	-	CLONING ARTIFACT	UNP P04849
C	486	SER	-	CLONING ARTIFACT	UNP P04849
C	487	LYS	-	CLONING ARTIFACT	UNP P04849
C	488	ILE	-	CLONING ARTIFACT	UNP P04849
C	489	TYR	-	CLONING ARTIFACT	UNP P04849
C	490	HIS	-	CLONING ARTIFACT	UNP P04849
C	491	ILE	-	CLONING ARTIFACT	UNP P04849
C	492	GLU	-	CLONING ARTIFACT	UNP P04849
C	493	ASN	-	CLONING ARTIFACT	UNP P04849
C	492	GLU	-	CLONING ARTIFACT	UNP P04849
C	495	ILE	-	CLONING ARTIFACT	UNP P04849
C	496	ALA	-	CLONING ARTIFACT	UNP P04849

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Chain	Residue	Modelled	Actual	Comment	Reference
C	497	ARG	-	CLONING ARTIFACT	UNP P04849
C	498	ILE	-	CLONING ARTIFACT	UNP P04849
C	499	LYS	-	CLONING ARTIFACT	UNP P04849
C	500	LYS	-	CLONING ARTIFACT	UNP P04849
C	501	LEU	-	CLONING ARTIFACT	UNP P04849
C	502	ILE	-	CLONING ARTIFACT	UNP P04849
C	503	GLY	-	CLONING ARTIFACT	UNP P04849
C	504	GLU	-	CLONING ARTIFACT	UNP P04849
C	505	ALA	-	CLONING ARTIFACT	UNP P04849
C	506	PRO	-	CLONING ARTIFACT	UNP P04849
C	507	GLY	-	CLONING ARTIFACT	UNP P04849
C	508	GLY	-	CLONING ARTIFACT	UNP P04849
C	509	ILE	-	CLONING ARTIFACT	UNP P04849
C	510	GLU	-	CLONING ARTIFACT	UNP P04849
C	511	GLY	-	CLONING ARTIFACT	UNP P04849
C	512	ARG	-	CLONING ARTIFACT	UNP P04849
C	513	HIS	-	EXPRESSION TAG	UNP P04849
C	514	HIS	-	EXPRESSION TAG	UNP P04849
C	513	HIS	-	EXPRESSION TAG	UNP P04849
C	514	HIS	-	EXPRESSION TAG	UNP P04849
C	515	HIS	-	EXPRESSION TAG	UNP P04849
C	516	HIS	-	EXPRESSION TAG	UNP P04849

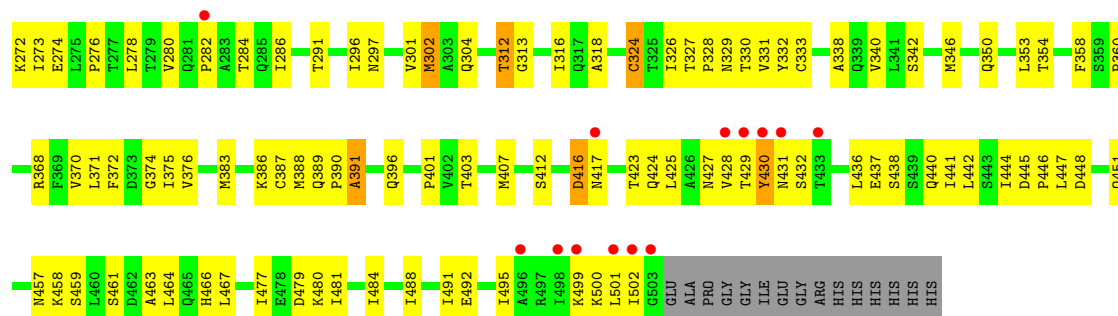
- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



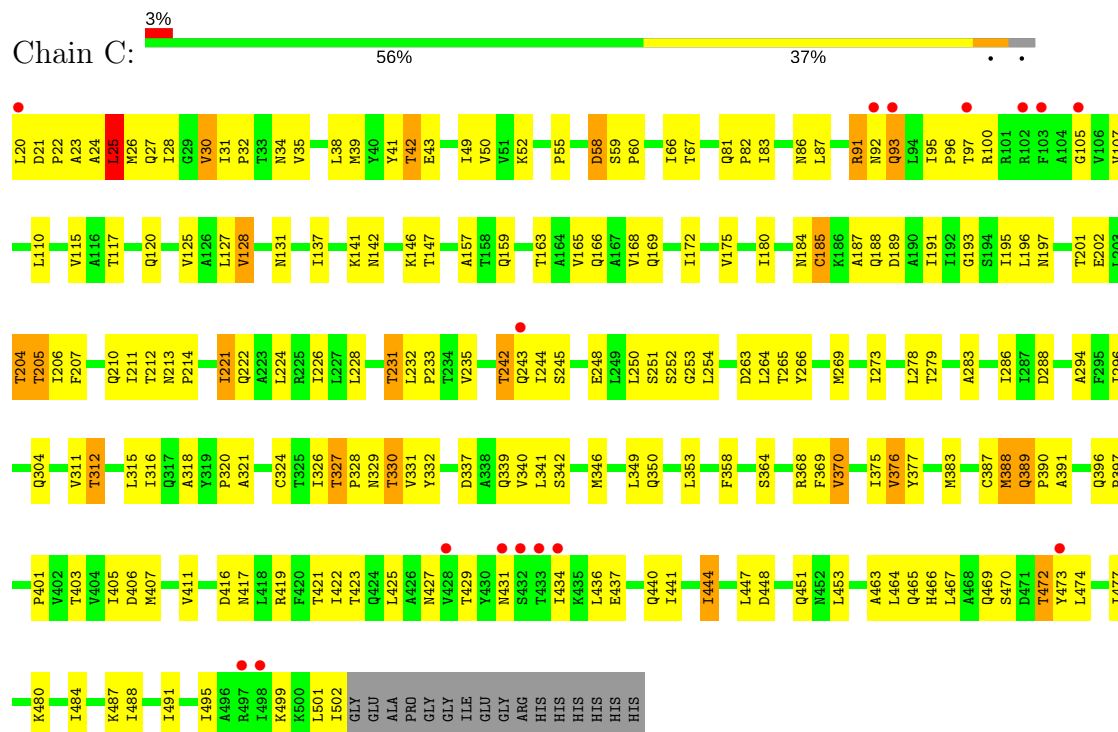
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	45	Total O 45 45	0	0
3	B	36	Total O 36 36	0	0
3	C	49	Total O 49 49	0	0



• Molecule 1: Fusion glycoprotein F0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	160.21Å 259.86Å 154.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.15 – 2.85 39.15 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.15-2.85) 99.7 (39.15-2.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.259 0.227 , 0.264	Depositor DCC
R_{free} test set	2251 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 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	0.35	0/3579	0.66	0/4891
1	B	0.35	0/3590	0.67	0/4916
1	C	0.37	0/3581	0.69	2/4904 (0.0%)
All	All	0.36	0/10750	0.67	2/14711 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	LEU	CA-CB-CG	6.30	129.79	115.30
1	C	25	LEU	N-CA-C	-5.63	95.79	111.00

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	3538	0	3643	227	0
1	B	3547	0	3619	240	0
1	C	3539	0	3616	218	0
2	A	56	0	52	1	0
2	B	56	0	52	4	0
2	C	56	0	52	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	45	0	0	3	0
3	B	36	0	0	5	0
3	C	49	0	0	2	0
All	All	10922	0	11034	629	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 29.

The worst 5 of 629 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:B:95:ILE:HG21	1:B:128:VAL:HG11	1.16	1.16
1:C:86:ASN:HD21	1:C:213:ASN:HA	1.08	1.15
1:C:31:ILE:HD13	1:C:370:VAL:HG11	1.40	1.04
1:B:165:VAL:HG21	1:B:231:THR:HG21	1.40	1.04
1:C:166:GLN:HG3	1:C:169:GLN:HB2	1.38	1.03

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	474/497 (95%)	431 (91%)	33 (7%)	10 (2%)	8	25
1	B	480/497 (97%)	422 (88%)	46 (10%)	12 (2%)	6	20
1	C	479/497 (96%)	443 (92%)	29 (6%)	7 (2%)	11	33
All	All	1433/1491 (96%)	1296 (90%)	108 (8%)	29 (2%)	8	26

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	92	ASN
1	A	416	ASP
1	B	185	CYS
1	B	324	CYS

5.3.2 Protein sidechains ⓘ

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	398/424 (94%)	379 (95%)	19 (5%)	28	59
1	B	397/424 (94%)	379 (96%)	18 (4%)	30	61
1	C	397/424 (94%)	375 (94%)	22 (6%)	24	53
All	All	1192/1272 (94%)	1133 (95%)	59 (5%)	27	58

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	ILE
1	B	312	THR
1	C	376	VAL
1	B	205	THR
1	B	221	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	258	GLN
1	B	424	GLN
1	C	440	GLN
1	B	297	ASN
1	B	440	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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$
2	NAG	A	1065	1	14,14,15	0.71	0	17,19,21	0.84	0
2	NAG	A	1073	1	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
2	NAG	A	1352	1	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
2	NAG	A	1457	1	14,14,15	0.64	0	17,19,21	1.00	1 (5%)
2	NAG	B	1065	1	14,14,15	0.65	0	17,19,21	0.67	0
2	NAG	B	1073	1	14,14,15	0.74	1 (7%)	17,19,21	0.65	0
2	NAG	B	1352	1	14,14,15	0.60	0	17,19,21	0.77	1 (5%)
2	NAG	B	1457	1	14,14,15	0.80	0	17,19,21	0.94	1 (5%)
2	NAG	C	1065	1	14,14,15	1.00	1 (7%)	17,19,21	1.24	1 (5%)
2	NAG	C	1073	1	14,14,15	0.75	1 (7%)	17,19,21	0.66	0
2	NAG	C	1352	1	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
2	NAG	C	1457	1	14,14,15	0.89	0	17,19,21	0.54	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
2	NAG	A	1065	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1073	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1352	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1457	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1065	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1073	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1352	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1457	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1065	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1073	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1352	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1457	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1073	NAG	C1-C2	2.01	1.55	1.52
2	C	1073	NAG	C1-C2	2.02	1.55	1.52
2	C	1065	NAG	O5-C5	2.35	1.48	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1065	NAG	C6-C5-C4	-3.43	104.88	112.99
2	A	1457	NAG	C4-C3-C2	-2.62	107.18	111.02
2	A	1352	NAG	C4-C3-C2	-2.45	107.43	111.02
2	B	1457	NAG	C4-C3-C2	-2.30	107.64	111.02
2	C	1352	NAG	C2-N2-C7	-2.11	119.87	122.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1457	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1352	NAG	1	0
2	B	1073	NAG	3	0
2	B	1457	NAG	1	0
2	C	1065	NAG	3	0
2	C	1073	NAG	5	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, 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	478/497 (96%)	-0.01	9 (1%) 66 64	26, 59, 111, 165	0
1	B	482/497 (96%)	0.11	22 (4%) 32 27	27, 63, 119, 158	0
1	C	481/497 (96%)	-0.05	16 (3%) 46 40	30, 55, 104, 180	0
All	All	1441/1491 (96%)	0.02	47 (3%) 46 40	26, 59, 112, 180	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	LEU	10.9
1	B	92	ASN	5.9
1	C	20	LEU	5.1
1	B	105	GLY	4.9
1	C	97	THR	4.8

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 carbohydrates 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, 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
2	NAG	C	1065	14/15	0.48	0.67	65,87,94,95	0
2	NAG	A	1065	14/15	0.71	0.40	65,87,94,95	0
2	NAG	B	1073	14/15	0.75	0.28	65,87,94,95	0
2	NAG	A	1352	14/15	0.78	0.38	65,87,94,95	0
2	NAG	B	1352	14/15	0.80	0.29	65,87,94,95	0
2	NAG	C	1457	14/15	0.80	0.34	65,87,94,95	0
2	NAG	B	1065	14/15	0.81	0.18	65,87,94,95	0
2	NAG	C	1073	14/15	0.81	0.27	65,87,94,95	0
2	NAG	A	1457	14/15	0.81	0.22	65,87,94,95	0
2	NAG	C	1352	14/15	0.83	0.32	65,87,94,95	0
2	NAG	B	1457	14/15	0.84	0.26	65,87,94,95	0
2	NAG	A	1073	14/15	0.94	0.17	41,54,57,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.