



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:11 AM BST

PDB ID : 5FQF
Title : The details of glycolipid glycan hydrolysis by the structural analysis of a family 123 glycoside hydrolase from *Clostridium perfringens*
Authors : Noach, I.; Pluvinaud, B.; Laurie, C.; Abe, K.T.; Alteen, M.; Vocadlo, D.J.; Boraston, A.B.
Deposited on : 2015-12-10
Resolution : 2.15 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 ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

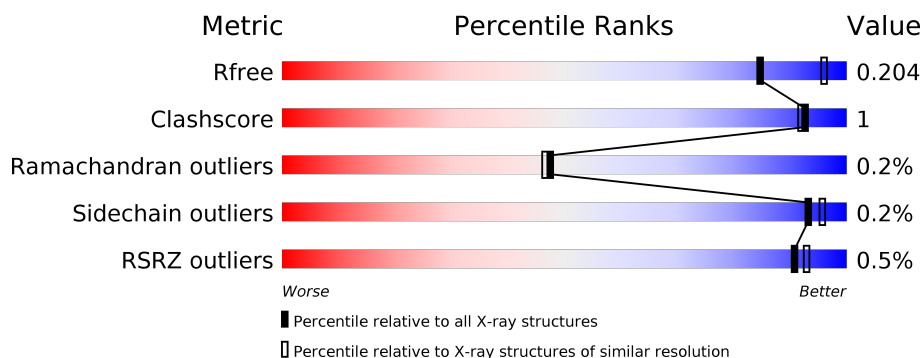
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	610	
1	B	610	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10495 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 BETA-N-ACETYLGALACTOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	10	12	0
			4814	3061	789	949	15			
1	B	580	Total	C	N	O	S	20	9	0
			4769	3037	789	929	14			

There are 46 discrepancies between the modelled and reference sequences:

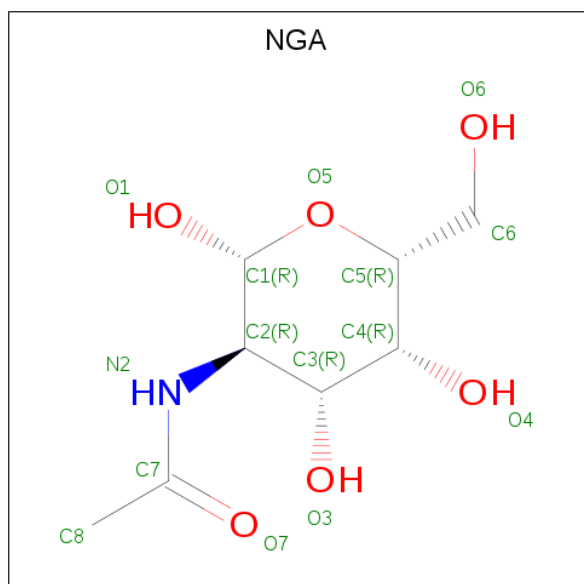
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP A0A0H2YNR7
A	-21	GLY	-	expression tag	UNP A0A0H2YNR7
A	-20	SER	-	expression tag	UNP A0A0H2YNR7
A	-19	SER	-	expression tag	UNP A0A0H2YNR7
A	-18	HIS	-	expression tag	UNP A0A0H2YNR7
A	-17	HIS	-	expression tag	UNP A0A0H2YNR7
A	-16	HIS	-	expression tag	UNP A0A0H2YNR7
A	-15	HIS	-	expression tag	UNP A0A0H2YNR7
A	-14	HIS	-	expression tag	UNP A0A0H2YNR7
A	-13	HIS	-	expression tag	UNP A0A0H2YNR7
A	-12	SER	-	expression tag	UNP A0A0H2YNR7
A	-11	SER	-	expression tag	UNP A0A0H2YNR7
A	-10	GLY	-	expression tag	UNP A0A0H2YNR7
A	-9	LEU	-	expression tag	UNP A0A0H2YNR7
A	-8	VAL	-	expression tag	UNP A0A0H2YNR7
A	-7	PRO	-	expression tag	UNP A0A0H2YNR7
A	-6	ARG	-	expression tag	UNP A0A0H2YNR7
A	-5	GLY	-	expression tag	UNP A0A0H2YNR7
A	-4	SER	-	expression tag	UNP A0A0H2YNR7
A	-3	HIS	-	expression tag	UNP A0A0H2YNR7
A	-2	MET	-	expression tag	UNP A0A0H2YNR7
A	-1	ALA	-	expression tag	UNP A0A0H2YNR7
A	0	SER	-	expression tag	UNP A0A0H2YNR7
B	-22	MET	-	expression tag	UNP A0A0H2YNR7
B	-21	GLY	-	expression tag	UNP A0A0H2YNR7

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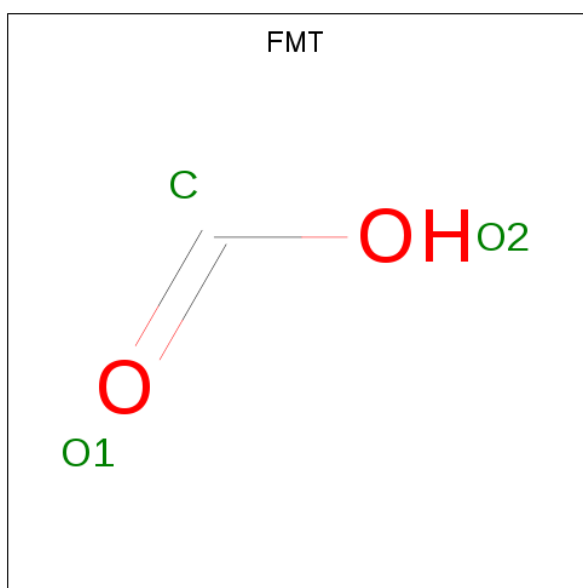
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP A0A0H2YNR7
B	-19	SER	-	expression tag	UNP A0A0H2YNR7
B	-18	HIS	-	expression tag	UNP A0A0H2YNR7
B	-17	HIS	-	expression tag	UNP A0A0H2YNR7
B	-16	HIS	-	expression tag	UNP A0A0H2YNR7
B	-15	HIS	-	expression tag	UNP A0A0H2YNR7
B	-14	HIS	-	expression tag	UNP A0A0H2YNR7
B	-13	HIS	-	expression tag	UNP A0A0H2YNR7
B	-12	SER	-	expression tag	UNP A0A0H2YNR7
B	-11	SER	-	expression tag	UNP A0A0H2YNR7
B	-10	GLY	-	expression tag	UNP A0A0H2YNR7
B	-9	LEU	-	expression tag	UNP A0A0H2YNR7
B	-8	VAL	-	expression tag	UNP A0A0H2YNR7
B	-7	PRO	-	expression tag	UNP A0A0H2YNR7
B	-6	ARG	-	expression tag	UNP A0A0H2YNR7
B	-5	GLY	-	expression tag	UNP A0A0H2YNR7
B	-4	SER	-	expression tag	UNP A0A0H2YNR7
B	-3	HIS	-	expression tag	UNP A0A0H2YNR7
B	-2	MET	-	expression tag	UNP A0A0H2YNR7
B	-1	ALA	-	expression tag	UNP A0A0H2YNR7
B	0	SER	-	expression tag	UNP A0A0H2YNR7

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 15 8 1 6	0	0
2	A	1	Total C N O 15 8 1 6	0	0
2	B	1	Total C N O 15 8 1 6	0	0
2	B	1	Total C N O 15 8 1 6	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0

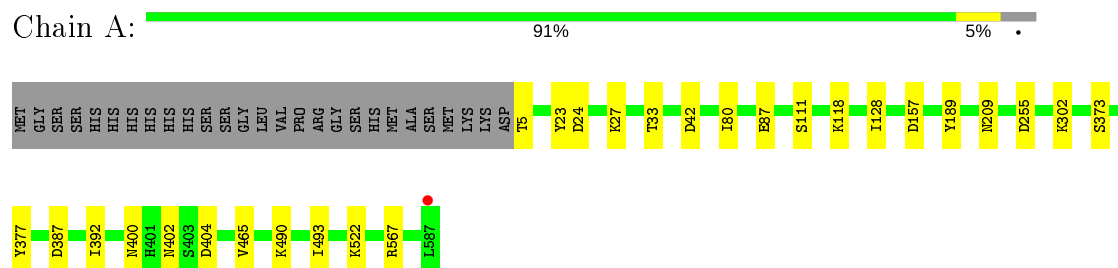
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	446	Total O 446 446	0	0
4	B	361	Total O 361 361	0	0

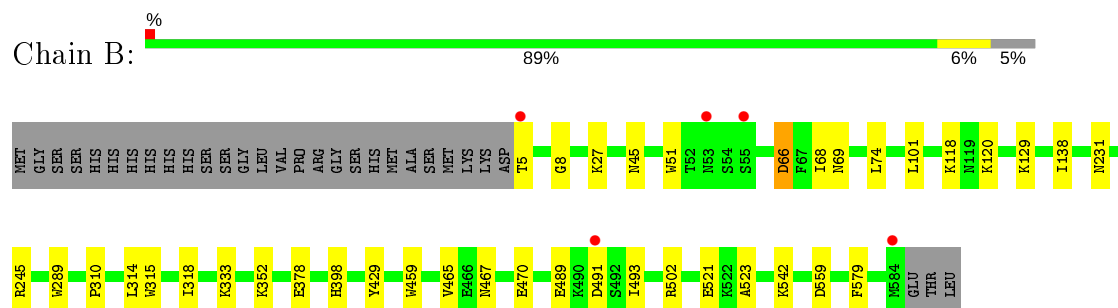
3 Residue-property plots

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: BETA-N-ACETYL GALACTOSAMINIDASE



• Molecule 1: BETA-N-ACETYL GALACTOSAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.03Å 114.79Å 134.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.37 – 2.15 44.86 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (87.37-2.15) 99.8 (44.86-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.147 , 0.198 0.158 , 0.204	Depositor DCC
R_{free} test set	3571 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10495	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: FMT, NGA

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	0.92	5/4950 (0.1%)	0.90	10/6727 (0.1%)
1	B	0.96	7/4901 (0.1%)	0.93	13/6657 (0.2%)
All	All	0.94	12/9851 (0.1%)	0.91	23/13384 (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
1	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	521	GLU	CD-OE1	-18.82	1.04	1.25
1	B	120	LYS	CD-CE	-13.61	1.17	1.51
1	A	522	LYS	CD-CE	-13.56	1.17	1.51
1	A	118	LYS	CD-CE	-12.71	1.19	1.51
1	B	352	LYS	CD-CE	-12.35	1.20	1.51
1	B	27	LYS	CG-CD	-7.29	1.27	1.52
1	A	302	LYS	CG-CD	-7.14	1.28	1.52
1	B	129	LYS	CD-CE	-7.03	1.33	1.51
1	B	118	LYS	CD-CE	-6.64	1.34	1.51
1	B	489	GLU	CD-OE2	-5.74	1.19	1.25
1	A	111	SER	CB-OG	-5.53	1.35	1.42
1	A	87	GLU	CD-OE2	-5.50	1.19	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	GLU	OE1-CD-OE2	15.97	142.47	123.30
1	B	120	LYS	CG-CD-CE	14.21	154.54	111.90
1	B	521	GLU	CG-CD-OE2	-8.97	100.36	118.30
1	B	245	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	387	ASP	CB-CG-OD1	7.26	124.84	118.30
1	A	255	ASP	CB-CG-OD1	6.98	124.59	118.30
1	B	245	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	42	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	42	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	120	LYS	CD-CE-NZ	-6.55	96.63	111.70
1	B	502	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	567	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	27	LYS	CB-CG-CD	5.81	126.71	111.60
1	B	352	LYS	CG-CD-CE	5.63	128.79	111.90
1	A	404	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	387	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	101	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	302	LYS	CB-CG-CD	5.33	125.46	111.60
1	B	66	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	24	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	493	ILE	N-CA-C	-5.21	96.94	111.00
1	B	491	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	502	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	459	TRP	Peptide

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	4814	0	4551	9	0
1	B	4769	0	4538	16	0
2	A	30	0	30	1	0
2	B	30	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	8	2	0
3	B	21	0	7	0	0
4	A	446	0	0	5	1
4	B	361	0	0	3	0
All	All	10495	0	9164	28	1

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 1.

All (28) 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:493:ILE:O	1:B:493:ILE:HD12	1.98	0.64
1:B:559:ASP:HB3	4:B:2343:HOH:O	1.97	0.64
3:A:1595:FMT:C	4:A:2446:HOH:O	2.48	0.61
1:A:80:ILE:HD12	1:A:128:ILE:HG12	1.85	0.58
1:A:402:ASN:N	4:A:2349:HOH:O	2.34	0.57
1:B:467:ASN:ND2	1:B:470[B]:GLU:OE1	2.41	0.54
1:B:429:TYR:HB3	1:B:542:LYS:HB3	1.93	0.50
1:B:66:ASP:HB3	1:B:74:LEU:HD11	1.94	0.49
1:A:5:THR:N	4:A:2001:HOH:O	2.45	0.48
1:A:400:ASN:HB3	4:A:2349:HOH:O	2.13	0.47
1:B:333:LYS:NZ	4:B:2190:HOH:O	2.47	0.47
1:A:189:TYR:O	1:A:490:LYS:HE3	2.15	0.47
1:A:373:SER:O	1:A:392:ILE:HA	2.15	0.47
1:B:66:ASP:HB3	1:B:74:LEU:CD1	2.45	0.47
1:A:23:TYR:CE2	1:A:27:LYS:HD2	2.51	0.46
1:B:523:ALA:HB2	1:B:579:PHE:CD1	2.50	0.46
1:B:310:PRO:HA	1:B:315:TRP:CD2	2.51	0.45
3:A:1592:FMT:O1	4:A:2099:HOH:O	2.21	0.45
1:B:69:ASN:HA	1:B:138:ILE:O	2.17	0.45
1:B:378:GLU:HG2	1:B:398:HIS:O	2.17	0.45
1:A:33[B]:THR:HG22	1:A:157:ASP:HB2	2.00	0.44
2:A:1588:NGA:O7	2:A:1588:NGA:H1	2.16	0.44
1:B:314:LEU:HD11	1:B:318:ILE:HD11	1.99	0.44
1:B:231:ASN:HB2	1:B:289:TRP:CG	2.55	0.42
1:B:45:ASN:HB2	4:B:2007:HOH:O	2.20	0.42
1:A:377:TYR:CD1	1:A:377:TYR:C	2.94	0.41
1:B:8:GLY:HA3	1:B:51:TRP:CE2	2.55	0.41
1:B:68:ILE:CD1	1:B:74:LEU:HD13	2.51	0.41

All (1) 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)
4:A:2143:HOH:O	4:A:2318:HOH:O[3_554]	2.12	0.08

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	593/610 (97%)	577 (97%)	15 (2%)	1 (0%)	47	46
1	B	587/610 (96%)	570 (97%)	16 (3%)	1 (0%)	47	46
All	All	1180/1220 (97%)	1147 (97%)	31 (3%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	465	VAL
1	A	465	VAL

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	532/549 (97%)	531 (100%)	1 (0%)	93	96
1	B	525/549 (96%)	524 (100%)	1 (0%)	93	96
All	All	1057/1098 (96%)	1055 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	B	5	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	53	ASN
1	B	119	ASN

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](#)

19 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	$\# Z > 2$
3	FMT	B	1600	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1589	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1596	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NGA	B	1586	-	15,15,15	0.80	0	21,21,21	2.04	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	A	1591	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1591	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1587	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1595	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1588	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1600	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NGA	A	1589	-	15,15,15	1.21	2 (13%)	21,21,21	2.64	10 (47%)
3	FMT	A	1590	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1601	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1594	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NGA	A	1588	-	15,15,15	0.63	0	21,21,21	1.54	4 (19%)
3	FMT	B	1590	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1593	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NGA	B	1585	-	15,15,15	1.07	1 (6%)	21,21,21	1.75	5 (23%)
3	FMT	A	1592	-	0,2,2	0.00	-	0,1,1	0.00	-

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	NGA	A	1589	-	-	2/6/26/26	0/1/1/1
2	NGA	A	1588	-	-	2/6/26/26	0/1/1/1
2	NGA	B	1586	-	-	1/6/26/26	0/1/1/1
2	NGA	B	1585	-	-	2/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1585	NGA	C2-N2	2.88	1.50	1.45
2	A	1589	NGA	C1-C2	2.28	1.55	1.52
2	A	1589	NGA	C3-C2	2.27	1.57	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1589	NGA	C1-C2-C3	-7.07	100.90	110.54
2	B	1586	NGA	C1-C2-C3	-6.02	102.33	110.54
2	B	1585	NGA	O5-C1-C2	5.05	114.59	109.52
2	A	1589	NGA	O7-C7-N2	4.37	129.98	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1589	NGA	O1-C1-C2	4.14	117.81	109.22
2	A	1588	NGA	O5-C1-C2	4.03	113.56	109.52
2	A	1589	NGA	C1-C2-N2	3.48	114.76	110.73
2	B	1586	NGA	O5-C1-C2	-3.10	106.40	109.52
2	A	1589	NGA	O3-C3-C2	2.88	115.46	109.66
2	B	1585	NGA	O1-C1-C2	-2.85	103.29	109.22
2	B	1586	NGA	O1-C1-C2	2.80	115.04	109.22
2	A	1589	NGA	C8-C7-N2	-2.78	111.39	116.10
2	A	1588	NGA	C8-C7-N2	2.58	120.46	116.10
2	A	1589	NGA	O5-C1-C2	-2.52	106.98	109.52
2	A	1589	NGA	C1-O5-C5	-2.51	108.92	113.66
2	A	1589	NGA	C2-N2-C7	2.45	129.13	123.18
2	B	1586	NGA	O7-C7-C8	-2.37	117.66	122.06
2	B	1585	NGA	C6-C5-C4	2.33	118.47	113.00
2	B	1586	NGA	C1-C2-N2	2.30	113.39	110.73
2	B	1586	NGA	O7-C7-N2	2.28	126.14	121.95
2	A	1588	NGA	C1-O5-C5	-2.22	109.47	113.66
2	B	1585	NGA	C1-O5-C5	-2.21	109.49	113.66
2	B	1585	NGA	O7-C7-C8	-2.21	117.96	122.06
2	A	1588	NGA	C3-C4-C5	-2.12	106.46	110.24
2	A	1589	NGA	C3-C2-N2	2.04	114.46	110.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1589	NGA	C4-C5-C6-O6
2	A	1589	NGA	O5-C5-C6-O6
2	B	1585	NGA	C1-C2-N2-C7
2	B	1586	NGA	O5-C5-C6-O6
2	A	1588	NGA	C1-C2-N2-C7
2	B	1585	NGA	C3-C2-N2-C7
2	A	1588	NGA	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1595	FMT	1	0
2	A	1588	NGA	1	0
3	A	1592	FMT	1	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	583/610 (95%)	-0.74	1 (0%)	95 96	11, 18, 35, 58	5 (0%)
1	B	580/610 (95%)	-0.52	5 (0%)	84 88	12, 21, 41, 65	10 (1%)
All	All	1163/1220 (95%)	-0.63	6 (0%)	91 93	11, 20, 39, 65	15 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	587	LEU	3.0
1	B	5	THR	2.4
1	B	53	ASN	2.4
1	B	491	ASP	2.3
1	B	584	MET	2.1
1	B	55	SER	2.1

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, 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
3	FMT	B	1600	3/3	0.70	0.32	48,48,56,59	0
3	FMT	A	1594	3/3	0.79	0.14	49,49,52,53	0
3	FMT	B	1589	3/3	0.80	0.16	50,50,51,52	0
2	NGA	A	1589	15/15	0.84	0.21	37,49,57,57	0
3	FMT	A	1591	3/3	0.88	0.14	45,45,48,56	0
3	FMT	A	1600	3/3	0.88	0.12	44,44,49,50	0
2	NGA	B	1586	15/15	0.89	0.24	44,51,56,58	0
3	FMT	A	1596	3/3	0.91	0.16	44,44,49,50	0
3	FMT	A	1593	3/3	0.92	0.08	43,43,44,46	0
3	FMT	B	1588	3/3	0.93	0.09	49,49,50,53	0
3	FMT	B	1601	3/3	0.93	0.10	49,49,50,51	0
3	FMT	A	1595	3/3	0.94	0.08	24,24,25,32	0
3	FMT	B	1591	3/3	0.94	0.14	38,38,39,40	0
3	FMT	A	1590	3/3	0.94	0.08	28,28,29,31	0
3	FMT	B	1590	3/3	0.95	0.11	32,32,33,34	0
3	FMT	A	1592	3/3	0.96	0.12	34,34,39,41	0
2	NGA	B	1585	15/15	0.97	0.11	12,13,15,16	0
2	NGA	A	1588	15/15	0.97	0.08	12,15,17,19	0
3	FMT	B	1587	3/3	0.98	0.07	26,26,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.