

wwPDB X-ray Structure Validation Summary Report (i)

Aug 19, 2023 – 07:09 PM EDT

PDB ID	:	2F9N
Title	:	Crystal Structure of the Recombinant Human Alpha I Tryptase Mutant
		m K192Q/D216G in Complex with Leupeptin
Authors	:	Rohr, K.B.; Selwood, T.; Marquardt, U.; Huber, R.; Schechter, N.M.; Bode,
		W.; Than, M.E.
Deposited on	:	2005-12-06
Resolution	:	1.60 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 (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:

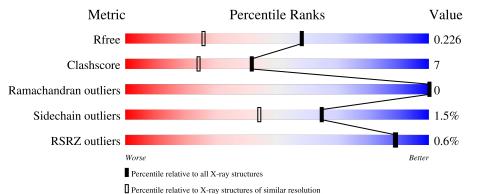
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.60 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	А	245	.% 87%	11%	
1	В	245		12%	•
1	С	245	86%	13%	•
1	D	245	87%	11%	••
2	Е	4	75%	25%	



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Mol	Chain	Length	Quality of chai	in
2	F	4	75%	25%
2	G	4	50%	50%
2	Н	4	50%	50%
3	Ι	4	75%	25%
3	J	4	100%	

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
5	NAG	D	1004	-	-	-	Х



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9588 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	042	Total	С	Ν	0	S	20	13	0
	А	243	2033	1304	351	364	14	30		0
1	В	243	Total	С	Ν	0	S	28	13	0
	ГБ	240	2029	1300	354	361	14	20		0
1	С	C 243	Total	С	Ν	0	S	30	12	0
			2027	1298	350	365	14	- 50	12	0
1	D	949	Total	С	Ν	0	S	22	15	0
	243	2049	1311	359	365	14	33	15	U	

• Molecule 1 is a protein called alpha I tryptase.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	59	VAL	LEU	engineered mutation	UNP P15157
А	186	SER	THR	variant	UNP P15157
А	187	GLN	ARG	variant	UNP P15157
A	192	GLN	LYS	engineered mutation	UNP P15157
А	216	GLY	ASP	engineered mutation	UNP P15157
В	59	VAL	LEU	engineered mutation	UNP P15157
В	186	SER	THR	variant	UNP P15157
В	187	GLN	ARG	variant	UNP P15157
В	192	GLN	LYS	engineered mutation	UNP P15157
В	216	GLY	ASP	engineered mutation	UNP P15157
С	59	VAL	LEU	engineered mutation	UNP P15157
С	186	SER	THR	variant	UNP P15157
С	187	GLN	ARG	variant	UNP P15157
С	192	GLN	LYS	engineered mutation	UNP P15157
С	216	GLY	ASP	engineered mutation	UNP P15157
D	59	VAL	LEU	engineered mutation	UNP P15157
D	186	SER	THR	variant	UNP P15157
D	187	GLN	ARG	variant	UNP P15157
D	192	GLN	LYS	engineered mutation	UNP P15157
D	216	GLY	ASP	engineered mutation	UNP P15157



Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
Е	4	Total C N O	0	0	0
F	4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	0	0
G	4	Total C N O	0	0	0
			-		
Н	4		0	0	0
-	E F G	E 4 F 4 G 4	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$

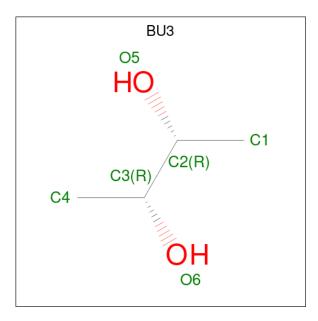
• Molecule 2 is a protein called Leupeptin.

• Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-be ta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyr anose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Ι	4	Total C N O 48 28 2 18	4	0	0
3	J	4	Total C N O 48 28 2 18	1	0	0

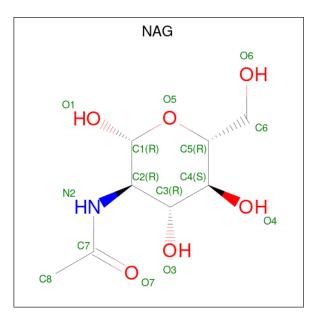
• Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: $C_4H_{10}O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 4 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 4 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	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
5	В	1	Total C N C 14 8 1 5		0
5	D	1	Total C N C 14 8 1 5	6	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	293	Total O 294 294	0	1
6	В	294	Total O 295 295	0	1
6	С	294	Total O 295 295	0	1



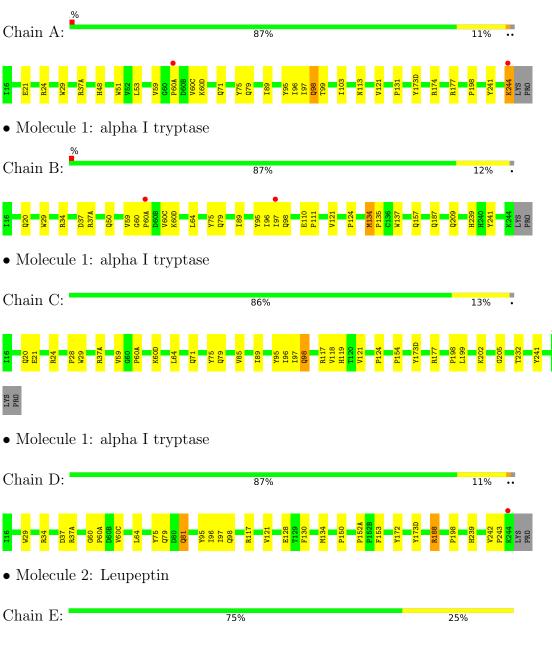
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	272	Total O 273 273	0	1
6	Е	7	Total O 7 7	0	0
6	F	6	Total O 6 6	0	0
6	G	6	Total O 6 6	0	0
6	Н	6	Total O 6 6	0	0



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: alpha I tryptase





• Molecule 2: Leupeptin

Chain F:	75%		25%
ACE301 L302 L303 R304 R304			
• Molecule 2: Leupeptin	1		
Chain G:	50%	50%	
ACE301 1.332 1.332 1.332 1.332 1.3324			
• Molecule 2: Leupeptin	1		
Chain H:	50%	50%	
ACE301 [1302 [1303 R304 R304			

 $\bullet \ Molecule \ 3: \ alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)] \\ 2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-6)] \\ 3-acetamido-2-deoxy-beta-D-glucopyranose \ (1-$

Chain I:	75%	25%
MAG1 FUG3 FUG4		

Chain J:

100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.31Å 88.57Å 163.37Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 - 1.60	Depositor
Resolution (A)	19.92 - 1.60	EDS
% Data completeness	98.8 (19.90-1.60)	Depositor
(in resolution range)	99.0 (19.92-1.60)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.74 (at 1.60\AA)	Xtriage
Refinement program	CNS 1.1	Depositor
D D.	0.190 , 0.236	Depositor
R, R_{free}	0.184 , 0.226	DCC
R_{free} test set	7659 reflections (4.89%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 53.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.51, \langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9588	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 50.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5342e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.

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, FUC, ACE, AR7, BU3

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.55	0/2103	0.75	0/2880	
1	В	0.57	0/2100	0.75	0/2876	
1	С	0.56	0/2095	0.75	1/2869~(0.0%)	
1	D	0.55	0/2120	0.76	1/2902~(0.0%)	
2	Е	0.45	0/16	1.01	0/21	
2	F	0.43	0/16	0.72	0/21	
2	G	0.49	0/16	0.98	0/21	
2	Н	0.36	0/16	0.87	0/21	
All	All	0.56	0/8482	0.75	2/11611~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	81	GLN	N-CA-C	-5.13	97.14	111.00
1	С	199	LEU	N-CA-C	-5.08	97.30	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	А	2033	0	1954	30	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	2029	0	1942	33	0
1	С	2027	0	1945	35	0
1	D	2049	0	1960	33	0
2	Е	30	0	38	6	0
2	F	30	0	38	4	0
2	G	30	0	38	5	0
2	Н	30	0	38	2	0
3	Ι	48	0	43	0	0
3	J	48	0	43	0	0
4	А	6	0	10	0	0
4	В	6	0	10	0	0
4	\mathbf{C}	6	0	10	0	0
4	D	6	0	10	0	0
5	В	14	0	13	0	0
5	D	14	0	13	0	0
6	А	294	0	0	5	0
6	В	295	0	0	4	0
6	С	295	0	0	6	0
6	D	273	0	0	3	0
6	Е	7	0	0	0	0
6	F	6	0	0	0	0
6	G	6	0	0	0	0
6	Н	6	0	0	0	0
All	All	9588	0	8105	114	0

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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 7.

The worst 5 of 114 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:C:60(A)[B]:PRO:HG3	1:C:96:ILE:HG23	1.16	1.15
1:A:60(A)[B]:PRO:HG3	1:A:96:ILE:HG23	1.16	1.10
1:B:97:ILE:HD11	2:G:302:LEU:HB3	1.43	1.00
1:C:60(A)[B]:PRO:CG	1:C:96:ILE:HG23	1.93	0.97
1:A:60(A)[B]:PRO:CG	1:A:96:ILE:HG23	2.02	0.88

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	Perce	ntiles
1	А	254/245~(104%)	245~(96%)	9~(4%)	0	100	100
1	В	254/245~(104%)	245~(96%)	9~(4%)	0	100	100
1	С	253/245~(103%)	247 (98%)	6(2%)	0	100	100
1	D	256/245~(104%)	246~(96%)	10 (4%)	0	100	100
2	Ε	2/4~(50%)	1 (50%)	1 (50%)	0	100	100
2	F	2/4~(50%)	1 (50%)	1 (50%)	0	100	100
2	G	2/4~(50%)	1 (50%)	1 (50%)	0	100	100
2	Н	2/4~(50%)	1 (50%)	1 (50%)	0	100	100
All	All	1025/996~(103%)	987~(96%)	38 (4%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	223/213~(105%)	217~(97%)	6 (3%)	44 20		
1	В	221/213~(104%)	220 (100%)	1 (0%)	88 80		
1	\mathbf{C}	222/213~(104%)	219~(99%)	3~(1%)	67 47		
1	D	223/213~(105%)	219~(98%)	4(2%)	59 36		
2	Ε	2/2~(100%)	2(100%)	0	100 100		
2	F	2/2~(100%)	2(100%)	0	100 100		



Mol	Chain	Analysed			
2	G	2/2~(100%)	2 (100%)	0	100 100
2	Н	2/2~(100%)	2(100%)	0	100 100
All	All	897/860~(104%)	883~(98%)	14 (2%)	65 41

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5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	20	GLN
1	С	98	GLN
1	D	198	PRO
1	D	188[A]	ARG
1	D	188[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	20	GLN
1	С	98	GLN
1	D	30	GLN
1	С	209	GLN
1	А	223	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)

4 non-standard protein/DNA/RNA residues 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).



Mal	Mol Type Chain	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
NIOI		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	AR7	Н	304	2	10,10,11	0.85	1 (10%)	9,11,13	0.41	0
2	AR7	Е	304	2	10,10,11	0.62	0	9,11,13	0.49	0
2	AR7	F	304	2	10,10,11	0.65	0	9,11,13	0.46	0
2	AR7	G	304	2	10,10,11	0.74	1 (10%)	9,11,13	0.66	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	AR7	Н	304	2	-	0/9/9/11	-
2	AR7	Е	304	2	-	0/9/9/11	-
2	AR7	F	304	2	-	0/9/9/11	-
2	AR7	G	304	2	-	0/9/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Н	304	AR7	C-CA	2.51	1.56	1.52
2	G	304	AR7	C-CA	2.22	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

8 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	\mathbf{ths}	Bond angles		
	Type	Ullaili	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Ι	1	3,1	$14,\!14,\!15$	0.84	0	17,19,21	0.70	0
3	FUC	Ι	2	3	10,10,11	0.98	0	$14,\!14,\!16$	0.79	1 (7%)
3	NAG	Ι	3	3	14,14,15	0.75	0	17,19,21	0.61	0
3	FUC	Ι	4	3	10,10,11	0.81	0	$14,\!14,\!16$	0.56	0
3	NAG	J	1	3,1	14,14,15	0.60	0	17,19,21	0.79	0
3	FUC	J	2	3	10,10,11	0.76	0	$14,\!14,\!16$	0.69	0
3	NAG	J	3	3	14,14,15	0.69	0	17,19,21	0.70	0
3	FUC	J	4	3	10,10,11	0.70	0	$14,\!14,\!16$	0.35	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	NAG	Ι	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	Ι	2	3	-	-	0/1/1/1
3	NAG	Ι	3	3	-	2/6/23/26	0/1/1/1
3	FUC	Ι	4	3	-	-	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1
3	NAG	J	3	3	-	2/6/23/26	0/1/1/1
3	FUC	J	4	3	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Ι	2	FUC	C1-C2-C3	2.20	112.37	109.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

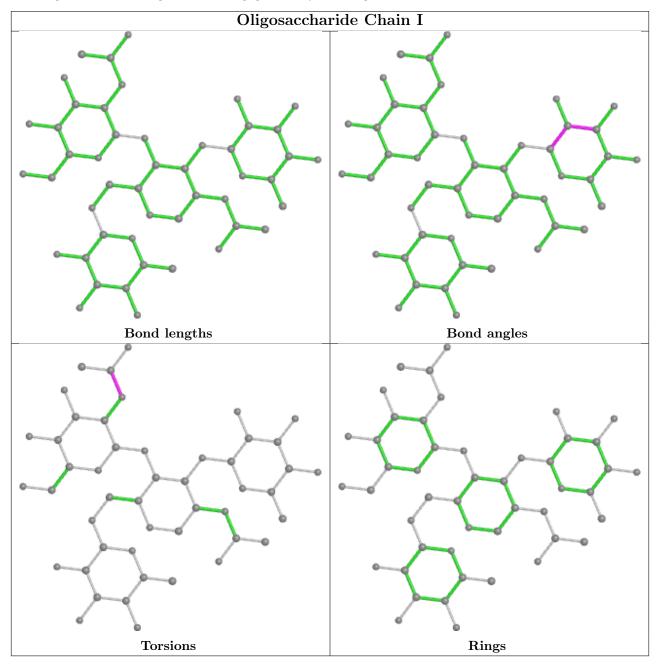
Mol	Chain	Res	Type	Atoms	
3	J	3	NAG	C8-C7-N2-C2	
3	J	3	NAG	O7-C7-N2-C2	
3	Ι	3	NAG	C8-C7-N2-C2	
3	Ι	3	NAG	O7-C7-N2-C2	

There are no ring outliers.

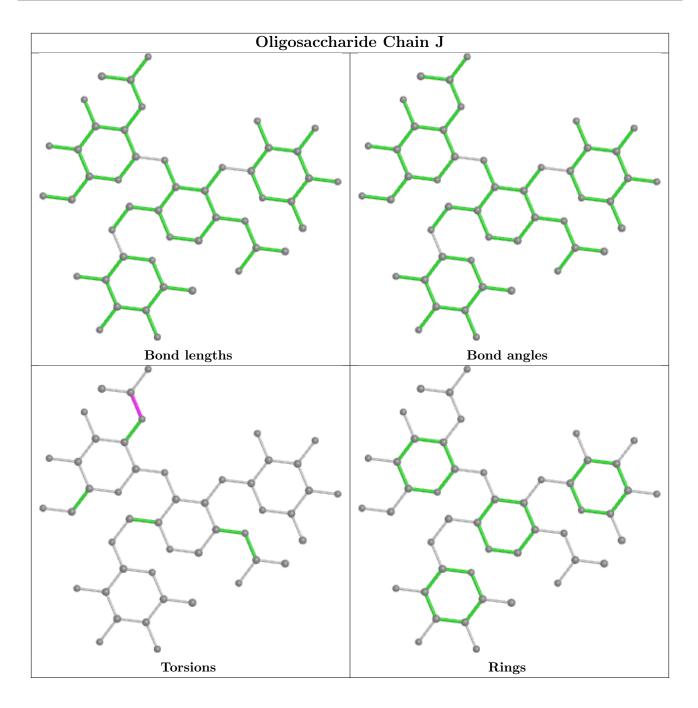


No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry (i)

6 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).



Mal	Mol Type	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
IVIOI		Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	BU3	С	2252	-	$4,\!5,\!5$	0.36	0	$6,\!6,\!6$	0.42	0
5	NAG	В	1004	1	$14,\!14,\!15$	0.97	0	17,19,21	1.09	2 (11%)
4	BU3	В	2251	-	$4,\!5,\!5$	0.45	0	6,6,6	0.39	0
4	BU3	D	2253	-	$4,\!5,\!5$	0.45	0	6,6,6	0.42	0
5	NAG	D	1004	1	14,14,15	0.85	0	17,19,21	0.74	0
4	BU3	А	2250	-	$4,\!5,\!5$	0.36	0	6,6,6	0.42	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	BU3	С	2252	-	-	0/4/4/4	-
5	NAG	В	1004	1	-	0/6/23/26	0/1/1/1
4	BU3	В	2251	-	-	0/4/4/4	-
4	BU3	D	2253	-	-	0/4/4/4	-
5	NAG	D	1004	1	-	0/6/23/26	0/1/1/1
4	BU3	A	2250	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	1004	NAG	C4-C3-C2	-2.91	106.76	111.02
5	В	1004	NAG	C2-N2-C7	-2.16	119.83	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{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	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	243/245~(99%)	-0.31	2 (0%) 86 86	12, 19, 36, 51	8 (3%)
1	В	243/245~(99%)	-0.40	2 (0%) 86 86	12, 18, 32, 40	8 (3%)
1	С	243/245~(99%)	-0.31	1 (0%) 92 92	12, 19, 36, 56	7 (2%)
1	D	243/245~(99%)	-0.31	1 (0%) 92 92	12, 20, 34, 47	10 (4%)
2	Ε	2/4~(50%)	-0.23	0 100 100	16, 16, 16, 30	0
2	F	2/4~(50%)	-0.56	0 100 100	15, 15, 15, 26	1 (50%)
2	G	2/4~(50%)	0.02	0 100 100	14, 14, 14, 28	0
2	Н	2/4~(50%)	0.01	0 100 100	18, 18, 18, 29	0
All	All	980/996~(98%)	-0.33	6 (0%) 89 89	12, 19, 36, 56	34 (3%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	244	LYS	2.8
1	А	244	LYS	2.7
1	D	244	LYS	2.5
1	А	60(A)[A]	PRO	2.3
1	В	97	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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	$B-factors(Å^2)$	Q<0.9
2	AR7	G	304	11/12	0.94	0.08	12,12,16,16	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	AR7	Н	304	11/12	0.94	0.09	$12,\!13,\!16,\!18$	0
2	AR7	Е	304	11/12	0.95	0.09	11,13,16,19	0
2	AR7	F	304	11/12	0.95	0.07	$10,\!13,\!15,\!18$	0

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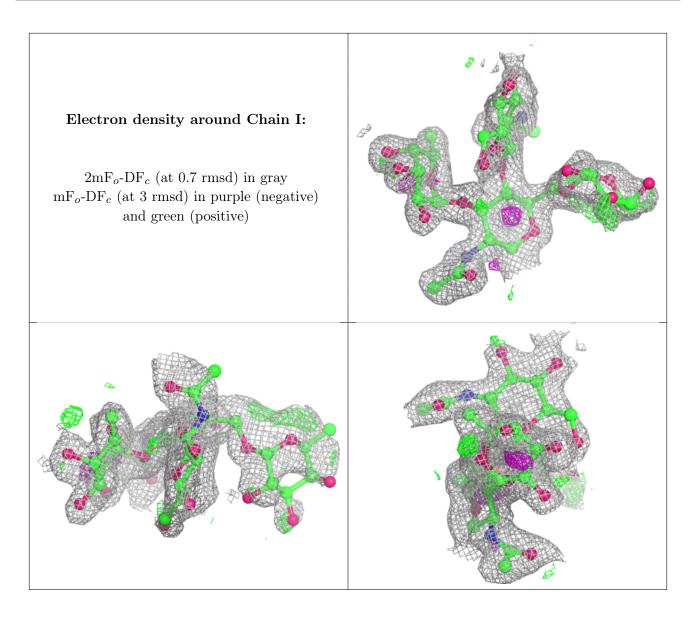
6.3 Carbohydrates (i)

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, 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.

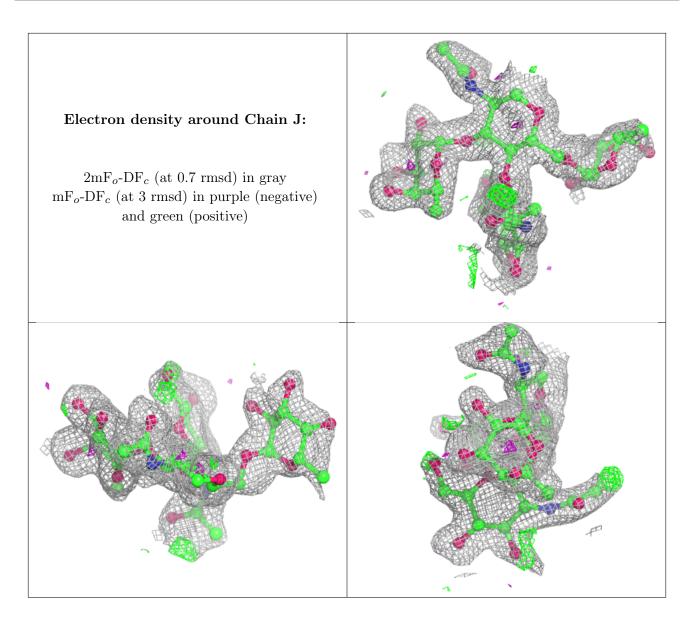
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	Ι	4	10/11	0.60	0.23	63,64,64,64	4
3	NAG	J	3	14/15	0.77	0.22	54,58,60,62	1
3	NAG	Ι	1	14/15	0.78	0.16	$38,\!45,\!57,\!62$	0
3	FUC	Ι	2	10/11	0.78	0.17	36,43,46,47	0
3	NAG	J	1	14/15	0.79	0.17	40,47,57,63	0
3	FUC	J	4	10/11	0.82	0.31	67,70,73,75	0
3	NAG	Ι	3	14/15	0.84	0.28	55,60,65,66	0
3	FUC	J	2	10/11	0.90	0.14	31,42,46,52	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, 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	$B-factors(Å^2)$	Q < 0.9
5	NAG	D	1004	14/15	0.32	0.41	63,67,70,72	6
5	NAG	В	1004	14/15	0.53	0.31	53,59,64,64	0
4	BU3	А	2250	6/6	0.91	0.10	20,24,25,29	0
4	BU3	С	2252	6/6	0.93	0.09	19,23,25,28	0
4	BU3	D	2253	6/6	0.97	0.07	21,25,28,30	0
4	BU3	В	2251	6/6	0.98	0.06	23,24,25,26	0



6.5 Other polymers (i)

There are no such residues in this entry.

