

wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 - 02:03 PM EST

PDB ID	:	3SEJ
Title	:	Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound
		to Secretor Lewis HBGA (LeB)
Authors	:	Shanker, S.; Choi, JM.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad,
		B.V.V.
Deposited on	:	2011-06-10
Resolution	:	3.04 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	:	2.36
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)	:	2.36

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 3.04 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	Similar resolution $(\#\text{Entries}, \text{resolution}, \text{range}(\text{\&}))$
	(#Entries)	(#Entries, resolution range(A))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	311	77%	21%	•••
1	В	311	77%	19%	•••
1	С	311	80%	17%	•
1	D	311	76%	21%	•••
1	Е	311	76%	20%	••



Mol	Chain	Length		Quality of chain	
1	F	311	7	7%	20% ••
1	G	311	74	%	23% ••
1	Н	311	74	%	21% • •
1	Ι	311	68%		21% · 9%
1	J	311	7	6%	21% ••
2	K	6	33%	50%	17%
2	L	6	17%	83%	
2	М	6	33%	67%	
2	Ν	6	17%	83%	
2	Ο	6	17% 33%		50%
2	Р	6	33%	50%	17%
2	Q	6	50%		50%
2	R	6	67%		33%

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	BGC	K	1	-	-	-	Х
2	GAL	K	2	-	-	-	Х
2	BGC	L	1	-	-	-	Х
2	GAL	L	2	-	-	-	Х
2	BGC	М	1	-	-	-	Х
2	GAL	М	2	-	-	-	Х
2	FUC	М	5	-	-	Х	-
2	FUC	М	6	-	-	Х	Х
2	BGC	N	1	-	-	-	Х
2	GAL	N	2	-	-	-	Х
2	FUC	N	5	-	-	Х	-
2	FUC	N	6	-	-	Х	-
2	BGC	0	1	-	-	-	Х
2	GAL	0	2	-	-	-	Х
2	BGC	Р	1	-	-	-	Х



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	Р	6	-	-	-	Х
2	BGC	Q	1	-	-	-	Х
2	FUC	Q	5	-	-	Х	-
2	BGC	R	1	-	-	Х	Х
2	GAL	R	2	-	-	Х	Х
2	FUC	R	6	-	-	Х	Х

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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24569 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	300	Total	С	Ν	0	S	0	0	0
1	Л	509	2403	1517	415	461	10	0	0	0
1	В	307	Total	С	Ν	Ο	\mathbf{S}	0	Ο	0
1	D	301	2382	1505	407	460	10	0	0	0
1	С	311	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	U	511	2416	1524	417	465	10	0	0	0
1	Л	307	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	D	301	2386	1507	410	459	10	0	0	0
1	E	309	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1		005	2406	1518	415	463	10	0	0	0
1	F	308	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
-	1	300	2393	1511	411	461	10	0	0	0
1	G	308	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	ŭ	300	2380	1505	407	458	10	0	0	0
1	н	300	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	11	500	2291	1456	393	432	10	0	0	0
1	т	284	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	1	201	2128	1347	371	402	8		0	0
1	Т	307	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	J	501	2383	1506	410	457	10	0	U	U

• Molecule 1 is a protein called Capsid.

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
А	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
А	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
В	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
В	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
В	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
С	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
С	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
C	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8



Chain	Residue	Modelled	Actual	Comment	Reference
D	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
D	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
D	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
Е	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
Е	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
Е	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
F	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
F	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
F	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
G	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
G	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
G	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
Н	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
Н	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
Н	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
Ι	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
Ι	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
Ι	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
J	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
J	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
J	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	K	6	Total C N O	0	0	0
_		Ũ	68 38 1 29	Ũ	Ŭ	•
9	т	6	Total C N O	0	0	0
		0	68 38 1 29	0		0
0	м	6	Total C N O	0	0	0
	111	0	68 38 1 29			
0	N	6	Total C N O	0	0	0
	2 N	0	68 38 1 29	0	0	0
0	0	6	Total C N O	0	0	0
	0	U	68 38 1 29	U	0	U



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Р	6	Total C N O 68 38 1 29	0	0	0
2	Q	6	Total C N O 68 38 1 29	0	0	0
2	R	6	Total C N O 68 38 1 29	0	0	0

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• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	68	Total O 68 68	0	0
3	В	54	$\begin{array}{ccc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
3	С	53	Total O 53 53	0	0
3	D	57	Total O 57 57	0	0
3	Е	46	Total O 46 46	0	0
3	F	45	Total O 45 45	0	0
3	G	41	Total O 41 41	0	0
3	Н	36	Total O 36 36	0	0
3	Ι	18	Total O 18 18	0	0
3	J	39	Total O 39 39	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: Capsid



P385 GLU P385 ARC P386 ARC P399 K249 P411 P253 P412 P253 P413 P253 P414 P253 P445 P253 P445 P269 P445 P269 P445 P269 P445 P269 P445 P269 P445 P289 P445 P289 P445 P289 P445 P289 P446 P289 P446 P289 P446 P289 P446 P289 P446 P289 P446 P310 P446 P310 P446

V521 N522 Q523 L527 L527 M530 G531

 \bullet Molecule 1: Capsid



 \bullet Molecule 1: Capsid



• Molecule 1: Capsid





1377 1377 1377 961 1377 1377 961 1377 1377 961 1377 1377 961 1377 1377 961 1377 1377 961 1377 1388 961 1388 1388 963 1388 1388 964 1388 1388 964 1384 1384 964 1384 1384 944 1384 1384 944 1384 1384 944 1384 1384 944 1384 1384 944 1384 1384 944 1384 1384 944 1384 1384 944 1444 1334 944 1334 1334 944 1334 1334 944 1334 1334 144 1334 1334 144 1334 1334 144 1444 1334 <





 • Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose





 • Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose

83%

Chain L: 17%

BGC1 GAL2 NAG3 GAL4 FUC5 FUC5

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose

Chain M:	33%	67%

BGC1 GAL2 NAG3 GAL4 FUC5 FUC6

 • Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose

Chain N:	17%	83%
BGC1 GAL2 NAG3 GAL4 FUC5 FUC6		

• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose

Chain O:	17%	33%	50%
BGC1 GAL2 NAG3 GAL4 FUC5 FUC6			

 • Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose

Chain P:	33%	50%	17%
BGC1 GAL2 NAG3 GAL4 FUC5 FUC6			

 • Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopy ranose

α · α		
Chain Q:	50%	50%
0		



BGC1 GAL2 NAG3 GAL4 FUC5 FUC5

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

33%

Chain R: 67%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	242.74Å 339.78Å 125.02Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(Å)	49.38 - 3.04	Depositor
Resolution (A)	49.38 - 3.04	EDS
% Data completeness	99.7 (49.38-3.04)	Depositor
(in resolution range)	99.7 (49.38-3.04)	EDS
R_{merge}	0.14	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) > 1$	$2.51 (at 3.07 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
P. P.	0.166 , 0.223	Depositor
n, n_{free}	0.171 , 0.222	DCC
R_{free} test set	4924 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 32.2	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24569	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: FUC, GAL, NAG, BGC

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).

Mal	Chain	Bo	nd lengths	Bond angles	
MOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.90	0/2473	0.89	2/3384~(0.1%)
1	В	0.85	0/2452	0.82	1/3357~(0.0%)
1	С	0.89	3/2486~(0.1%)	0.83	2/3401~(0.1%)
1	D	0.84	0/2456	0.85	4/3361~(0.1%)
1	Е	0.86	0/2476	0.88	2/3388~(0.1%)
1	F	0.81	0/2463	0.83	1/3371~(0.0%)
1	G	0.80	0/2450	0.81	3/3355~(0.1%)
1	Н	0.80	0/2356	0.85	1/3225~(0.0%)
1	Ι	0.83	0/2188	0.78	2/2993~(0.1%)
1	J	0.83	0/2453	0.83	2/3357~(0.1%)
All	All	0.84	3/24253~(0.0%)	0.84	20/33192~(0.1%)

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	Ε	0	1
1	J	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	С	221	GLU	CB-CG	5.70	1.62	1.52
1	С	221	GLU	CG-CD	5.38	1.60	1.51
1	С	524	PHE	CE2-CZ	5.26	1.47	1.37

The worst 5 of 20 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Ι	346	GLY	N-CA-C	8.95	135.48	113.10
1	G	495	GLY	N-CA-C	6.98	130.54	113.10
1	В	334	LEU	CB-CG-CD1	-6.86	99.35	111.00
1	J	495	GLY	N-CA-C	6.66	129.75	113.10
1	G	496	TYR	N-CA-CB	-6.48	98.94	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Е	344	THR	Peptide
1	J	345	ARG	Sidechain

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	2403	0	2292	57	0
1	В	2382	0	2264	38	0
1	С	2416	0	2304	42	0
1	D	2386	0	2275	46	0
1	Е	2406	0	2297	46	0
1	F	2393	0	2282	56	0
1	G	2380	0	2263	66	0
1	Н	2291	0	2167	53	0
1	Ι	2128	0	1939	49	0
1	J	2383	0	2273	54	0
2	K	68	0	60	2	0
2	L	68	0	60	8	0
2	М	68	0	60	15	0
2	N	68	0	60	18	0
2	0	68	0	60	6	0
2	Р	68	0	60	6	0
2	Q	68	0	60	20	0
2	R	68	0	60	21	0
3	А	68	0	0	9	0
3	В	54	0	0	12	0
3	С	53	0	0	13	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	57	0	0	10	0
3	Е	46	0	0	13	0
3	F	45	0	0	15	0
3	G	41	0	0	8	0
3	Н	36	0	0	16	0
3	Ι	18	0	0	10	0
3	J	39	0	0	6	0
All	All	24569	0	22836	560	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 12.

The worst 5 of 560 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:J:345:ARG:HD3	2:Q:5:FUC:O3	1.40	1.20
1:J:345:ARG:HG2	1:J:345:ARG:HH21	1.07	1.18
1:H:231:ILE:HB	3:H:545:HOH:O	1.40	1.18
1:B:481:ASP:HB2	3:B:181:HOH:O	1.43	1.16
1:F:512:ASN:HB3	3:F:544:HOH:O	1.50	1.12

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	entiles
1	А	307/311~(99%)	293~(95%)	14 (5%)	0	100	100
1	В	305/311~(98%)	294 (96%)	11 (4%)	0	100	100
1	С	309/311~(99%)	294 (95%)	15 (5%)	0	100	100
1	D	305/311~(98%)	297 (97%)	8 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Ε	307/311~(99%)	290 (94%)	17 (6%)	0	100 100
1	F	306/311~(98%)	290~(95%)	16 (5%)	0	100 100
1	G	306/311~(98%)	295~(96%)	11 (4%)	0	100 100
1	Н	294/311~(94%)	278~(95%)	16 (5%)	0	100 100
1	Ι	274/311 (88%)	252 (92%)	20 (7%)	2(1%)	22 57
1	J	305/311~(98%)	295~(97%)	10 (3%)	0	100 100
All	All	3018/3110 (97%)	2878 (95%)	138 (5%)	2(0%)	51 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ι	425	THR
1	Ι	231	ILE

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	Perc	entiles
1	А	269/272~(99%)	253~(94%)	16 (6%)	19	51
1	В	268/272~(98%)	247 (92%)	21 (8%)	12	39
1	С	271/272~(100%)	248 (92%)	23 (8%)	10	36
1	D	268/272~(98%)	250 (93%)	18 (7%)	16	46
1	Е	271/272~(100%)	248 (92%)	23 (8%)	10	36
1	F	269/272~(99%)	252 (94%)	17 (6%)	18	49
1	G	266/272~(98%)	245 (92%)	21 (8%)	12	39
1	Н	249/272~(92%)	228 (92%)	21 (8%)	11	36
1	Ι	219/272~(80%)	199 (91%)	20 (9%)	9	32
1	J	267/272~(98%)	244 (91%)	23 (9%)	10	35
All	All	2617/2720~(96%)	2414 (92%)	203 (8%)	12	39



5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	F	484	ARG
1	Н	331	GLN
1	J	481	ASP
1	G	277	GLN
1	G	381	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Ι	469	GLN
1	J	390	GLN
1	D	310	ASN
1	D	306	GLN
1	J	398	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)

48 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 7	Turne	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	les
MOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	K	1	2	12,12,12	0.50	0	17,17,17	0.77	1 (5%)
2	GAL	K	2	2	11,11,12	0.37	0	$15,\!15,\!17$	0.89	0



Mal	T	Chain	Dec	T : 1-	Bo	ond leng	ths	В	ond ang	les
NIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	К	3	2	14,14,15	0.55	0	$17,\!19,\!21$	0.92	1 (5%)
2	GAL	К	4	2	11,11,12	0.32	0	$15,\!15,\!17$	0.83	0
2	FUC	K	5	2	10,10,11	0.43	0	$14,\!14,\!16$	0.84	0
2	FUC	K	6	2	10,10,11	0.42	0	14,14,16	0.84	0
2	BGC	L	1	2	12,12,12	0.53	0	$17,\!17,\!17$	1.53	4 (23%)
2	GAL	L	2	2	11,11,12	0.55	0	$15,\!15,\!17$	1.49	2 (13%)
2	NAG	L	3	2	14,14,15	0.98	1 (7%)	17,19,21	2.11	<mark>5 (29%)</mark>
2	GAL	L	4	2	11,11,12	2.01	3 (27%)	$15,\!15,\!17$	2.44	5 (33%)
2	FUC	L	5	2	10,10,11	1.86	4 (40%)	14,14,16	3.88	5 (35%)
2	FUC	L	6	2	10,10,11	1.68	3 (30%)	14,14,16	2.92	6 (42%)
2	BGC	М	1	2	12,12,12	0.48	0	17,17,17	0.96	1 (5%)
2	GAL	М	2	2	11,11,12	0.34	0	$15,\!15,\!17$	0.85	0
2	NAG	М	3	2	14,14,15	0.97	1 (7%)	17,19,21	2.39	3 (17%)
2	GAL	М	4	2	11,11,12	1.63	2 (18%)	$15,\!15,\!17$	2.50	4 (26%)
2	FUC	М	5	2	10,10,11	1.45	1 (10%)	14,14,16	3.54	4 (28%)
2	FUC	М	6	2	10,10,11	0.41	0	14,14,16	0.86	0
2	BGC	N	1	2	12,12,12	0.83	0	17,17,17	2.20	6 (35%)
2	GAL	Ν	2	2	11,11,12	0.70	0	15, 15, 17	1.95	3 (20%)
2	NAG	Ν	3	2	14,14,15	0.90	1 (7%)	17,19,21	2.53	2 (11%)
2	GAL	N	4	2	11,11,12	1.78	3 (27%)	15, 15, 17	3.01	6 (40%)
2	FUC	N	5	2	10,10,11	0.45	0	14,14,16	0.78	0
2	FUC	N	6	2	10,10,11	0.46	0	14,14,16	0.97	1 (7%)
2	BGC	0	1	2	12,12,12	1.16	1 (8%)	17,17,17	2.14	5 (29%)
2	GAL	0	2	2	11,11,12	1.08	1 (9%)	15, 15, 17	2.39	7 (46%)
2	NAG	0	3	2	14,14,15	1.00	1 (7%)	17,19,21	1.74	4 (23%)
2	GAL	0	4	2	11,11,12	2.06	2 (18%)	$15,\!15,\!17$	2.35	6 (40%)
2	FUC	0	5	2	10,10,11	0.60	0	14,14,16	0.98	0
2	FUC	0	6	2	10,10,11	0.40	0	14,14,16	0.83	0
2	BGC	Р	1	2	12,12,12	0.50	0	17,17,17	0.77	1 (5%)
2	GAL	Р	2	2	11,11,12	0.37	0	15,15,17	0.89	0
2	NAG	Р	3	2	14,14,15	0.53	0	17,19,21	0.92	0
2	GAL	P	4	2	11,11,12	0.33	0	15,15,17	0.83	0
2	FUC	Р	5	2	10,10,11	0.43	0	14,14,16	0.84	0
2	FUC	P	6	2	10,10,11	0.43	0	14,14,16	0.84	0
2	BGC	Q	1	2	12,12,12	0.50	0	17,17,17	0.77	1 (5%)
2	GAL	Q	2	2	11,11,12	0.38	0	$15,\!15,\!17$	0.90	1 (6%)
2	NAG	Q	3	2	14,14,15	0.55	0	17,19,21	0.92	1 (5%)



Mal	Type Chain Bes Li		Tink	Bond lengths			Bond angles			
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GAL	Q	4	2	11,11,12	0.33	0	15,15,17	0.83	0
2	FUC	Q	5	2	10,10,11	0.42	0	14,14,16	0.83	0
2	FUC	Q	6	2	10,10,11	0.42	0	14,14,16	0.84	0
2	BGC	R	1	2	12,12,12	0.49	0	17,17,17	0.77	1 (5%)
2	GAL	R	2	2	11,11,12	0.37	0	15,15,17	0.90	1 (6%)
2	NAG	R	3	2	14,14,15	0.54	0	17,19,21	0.91	0
2	GAL	R	4	2	11,11,12	0.32	0	15,15,17	0.83	0
2	FUC	R	5	2	10,10,11	0.42	0	14,14,16	0.84	0
2	FUC	R	6	2	10,10,11	0.42	0	14,14,16	0.83	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	BGC	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	_	0/2/19/22	0/1/1/1
2	NAG	K	3	2	-	2/6/23/26	0/1/1/1
2	GAL	K	4	2	-	2/2/19/22	0/1/1/1
2	FUC	K	5	2	-	-	0/1/1/1
2	FUC	K	6	2	-	-	0/1/1/1
2	BGC	L	1	2	-	2/2/22/22	0/1/1/1
2	GAL	L	2	2	-	2/2/19/22	0/1/1/1
2	NAG	L	3	2	-	2/6/23/26	0/1/1/1
2	GAL	L	4	2	-	1/2/19/22	0/1/1/1
2	FUC	L	5	2	-	-	0/1/1/1
2	FUC	L	6	2	-	-	0/1/1/1
2	BGC	М	1	2	-	2/2/22/22	0/1/1/1
2	GAL	М	2	2	-	0/2/19/22	0/1/1/1
2	NAG	М	3	2	-	0/6/23/26	0/1/1/1
2	GAL	М	4	2	-	2/2/19/22	0/1/1/1
2	FUC	М	5	2	-	-	0/1/1/1
2	FUC	М	6	2	-	-	0/1/1/1
2	BGC	Ν	1	2	-	2/2/22/22	0/1/1/1
2	GAL	N	2	2	-	1/2/19/22	0/1/1/1
2	NAG	Ν	3	2	-	0/6/23/26	0/1/1/1
2	GAL	N	4	2	-	2/2/19/22	0/1/1/1
2	FUC	N	5	2	-	-	0/1/1/1
2	FUC	N	6	2	-	-	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	0	1	2	-	2/2/22/22	0/1/1/1
2	GAL	0	2	2	_	0/2/19/22	0/1/1/1
2	NAG	0	3	2	-	2/6/23/26	0/1/1/1
2	GAL	0	4	2	-	2/2/19/22	0/1/1/1
2	FUC	0	5	2	-	-	0/1/1/1
2	FUC	0	6	2	-	-	0/1/1/1
2	BGC	Р	1	2	-	2/2/22/22	0/1/1/1
2	GAL	Р	2	2	-	2/2/19/22	0/1/1/1
2	NAG	Р	3	2	-	2/6/23/26	0/1/1/1
2	GAL	Р	4	2	-	0/2/19/22	0/1/1/1
2	FUC	Р	5	2	-	-	0/1/1/1
2	FUC	Р	6	2	-	-	0/1/1/1
2	BGC	Q	1	2	-	2/2/22/22	0/1/1/1
2	GAL	Q	2	2	-	2/2/19/22	0/1/1/1
2	NAG	Q	3	2	-	0/6/23/26	0/1/1/1
2	GAL	Q	4	2	-	1/2/19/22	0/1/1/1
2	FUC	Q	5	2	-	-	0/1/1/1
2	FUC	Q	6	2	-	-	0/1/1/1
2	BGC	R	1	2	-	0/2/22/22	0/1/1/1
2	GAL	R	2	2	-	2/2/19/22	0/1/1/1
2	NAG	R	3	2	-	0/6/23/26	0/1/1/1
2	GAL	R	4	2	-	1/2/19/22	0/1/1/1
2	FUC	R	5	2	-	-	0/1/1/1
2	FUC	R	6	2	-	-	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	4	GAL	O5-C1	-4.83	1.36	1.43
2	М	4	GAL	O5-C1	-4.19	1.37	1.43
2	М	5	FUC	O5-C1	-4.14	1.37	1.43
2	L	4	GAL	O5-C1	-4.09	1.37	1.43
2	0	4	GAL	O5-C5	-4.05	1.35	1.43

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	М	5	FUC	O5-C1-C2	-10.56	94.48	110.77
2	L	5	FUC	C6-C5-C4	-9.82	94.92	113.07
2	N	3	NAG	C6-C5-C4	-9.12	91.65	113.00



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	М	3	NAG	C6-C5-C4	-7.92	94.45	113.00
2	L	5	FUC	O5-C5-C4	-7.06	96.85	109.52

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	BGC	C4-C5-C6-O6
2	0	1	BGC	O5-C5-C6-O6
2	0	4	GAL	O5-C5-C6-O6
2	N	1	BGC	C4-C5-C6-O6
2	L	2	GAL	O5-C5-C6-O6

There are no ring outliers.

40 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	5	FUC	12	0
2	М	6	FUC	8	0
2	Ν	4	GAL	4	0
2	Ν	5	FUC	8	0
2	Q	4	GAL	3	0
2	М	2	GAL	2	0
2	0	1	BGC	4	0
2	Р	6	FUC	4	0
2	Ν	6	FUC	14	0
2	Κ	3	NAG	1	0
2	Q	6	FUC	5	0
2	R	5	FUC	5	0
2	М	5	FUC	8	0
2	Ν	3	NAG	4	0
2	Q	2	GAL	4	0
2	L	5	FUC	2	0
2	Р	1	BGC	1	0
2	Q	3	NAG	2	0
2	L	2	GAL	1	0
2	N	2	GAL	1	0
2	М	3	NAG	3	0
2	L	6	FUC	4	0
2	Q	1	BGC	2	0
2	0	3	NAG	2	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	М	1	BGC	2	0
2	0	2	GAL	1	0
2	R	4	GAL	3	0
2	K	6	FUC	2	0
2	L	1	BGC	2	0
2	R	6	FUC	14	0
2	Р	3	NAG	2	0
2	М	4	GAL	5	0
2	L	3	NAG	4	0
2	K	4	GAL	1	0
2	0	6	FUC	2	0
2	R	1	BGC	6	0
2	R	2	GAL	6	0
2	N	1	BGC	1	0
2	Р	4	GAL	3	0
2	R	3	NAG	2	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)

There are no ligands in this entry.

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>	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	309/311~(99%)	-0.74	0 100 100	10, 22, 54, 90	0
1	В	307/311~(98%)	-0.73	0 100 100	15, 26, 51, 65	0
1	С	311/311~(100%)	-0.57	0 100 100	13, 27, 49, 64	0
1	D	307/311~(98%)	-0.59	1 (0%) 94 83	11, 27, 59, 82	0
1	Ε	309/311~(99%)	-0.62	0 100 100	15, 28, 60, 74	0
1	F	308/311~(99%)	-0.55	0 100 100	20, 39, 68, 83	0
1	G	308/311~(99%)	-0.53	1 (0%) 94 83	22, 38, 63, 104	0
1	Н	300/311~(96%)	-0.33	0 100 100	17, 41, 79, 109	0
1	Ι	284/311~(91%)	0.87	33 (11%) 4 1	51, 81, 110, 140	0
1	J	307/311~(98%)	-0.63	0 100 100	17, 33, 62, 79	0
All	All	3050/3110 (98%)	-0.46	35 (1%) 80 56	10, 33, 83, 140	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	296	THR	4.1
1	Ι	300	THR	3.9
1	Ι	411	ARG	3.2
1	Ι	297	GLN	3.2
1	Ι	293	ILE	3.0

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, 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	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	BGC	L	1	12/12	0.52	0.74	124,130,130,130	0
2	GAL	М	2	11/12	0.58	0.54	108,115,118,118	0
2	BGC	М	1	12/12	0.60	0.58	122,125,126,126	0
2	BGC	K	1	12/12	0.60	0.57	126,130,130,131	0
2	BGC	Q	1	12/12	0.64	0.60	113,116,117,117	0
2	GAL	L	2	11/12	0.65	0.46	111,116,119,120	0
2	GAL	N	2	11/12	0.66	0.44	111,115,119,120	0
2	BGC	R	1	12/12	0.66	0.64	129,133,133,133	0
2	FUC	М	6	10/11	0.69	0.40	91,93,94,95	0
2	GAL	Κ	2	11/12	0.70	0.48	113,119,122,123	0
2	NAG	Q	3	14/15	0.70	0.32	97,103,106,106	0
2	FUC	Р	6	10/11	0.70	0.49	$119,\!120,\!121,\!121$	0
2	BGC	Р	1	12/12	0.71	0.41	134,136,136,136	0
2	GAL	Q	2	11/12	0.71	0.36	110,113,114,114	0
2	GAL	Р	2	11/12	0.72	0.30	126,130,131,132	0
2	BGC	0	1	12/12	0.72	0.64	105,109,109,109	0
2	FUC	N	6	10/11	0.74	0.38	97,99,99,99	0
2	FUC	R	6	10/11	0.75	0.49	107,108,109,109	0
2	GAL	0	2	11/12	0.77	0.58	93,97,101,101	0
2	BGC	N	1	12/12	0.77	0.58	123,126,126,127	0
2	GAL	R	2	11/12	0.77	0.47	119,122,125,126	0
2	FUC	K	6	10/11	0.77	0.35	99,100,101,101	0
2	GAL	Р	4	11/12	0.78	0.39	108,112,113,114	0
2	FUC	L	6	10/11	0.78	0.30	92,96,97,98	0
2	GAL	М	4	11/12	0.79	0.33	83,88,89,90	0
2	FUC	Q	5	10/11	0.79	0.25	70,74,76,79	0
2	FUC	Q	6	10/11	0.79	0.37	100,101,102,102	0
2	NAG	М	3	14/15	0.81	0.38	93,97,101,103	0
2	NAG	L	3	14/15	0.81	0.37	98,102,104,106	0
2	GAL	N	4	11/12	0.82	0.36	92,94,96,96	0
2	NAG	P	3	14/15	0.82	0.43	117,121,123,124	0
2	NAG	R	3	14/15	0.82	0.44	104,111,112,114	0
2	FUC	N	5	10/11	0.82	0.29	84,87,88,89	0
2	NAG	0	3	14/15	0.83	0.40	79,83,86,88	0
2	FUC	K	5	10/11	0.83	0.25	74,77,78,80	0
2	NAG	K	3	14/15	0.83	0.46	$98,\!104,\!107,\!108$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	FUC	R	5	10/11	0.84	0.29	83,84,86,88	0
2	NAG	N	3	14/15	0.84	0.41	97,102,105,106	0
2	GAL	Q	4	11/12	0.85	0.25	85,96,97,97	0
2	GAL	R	4	11/12	0.85	0.30	92,96,99,99	0
2	FUC	0	6	10/11	0.86	0.32	73,75,76,77	0
2	FUC	L	5	10/11	0.87	0.19	71,72,75,78	0
2	FUC	М	5	10/11	0.87	0.27	73,74,77,79	0
2	FUC	0	5	10/11	0.87	0.22	57,61,62,63	0
2	GAL	K	4	11/12	0.88	0.34	84,91,92,92	0
2	GAL	L	4	11/12	0.88	0.30	85,91,93,93	0
2	GAL	0	4	11/12	0.90	0.29	68,72,74,75	0
2	FUC	Р	5	10/11	0.91	0.25	100,101,102,104	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

