



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:54 am GMT

PDB ID : 3SEJ
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to Secretor Lewis HBGA (LeB)
Authors : Shanker, S.; Choi, J.-M.; 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

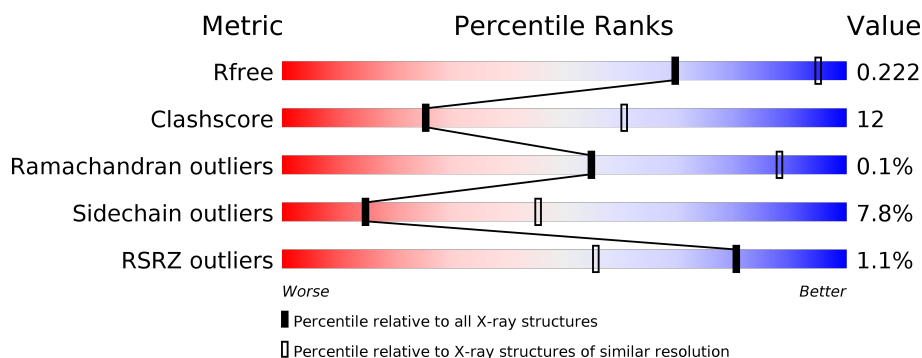
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2176 (3.08-3.00)
Clashscore	112137	2542 (3.08-3.00)
Ramachandran outliers	110173	2458 (3.08-3.00)
Sidechain outliers	110143	2461 (3.08-3.00)
RSRZ outliers	101464	2202 (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 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	311	 77% 21% ..
1	B	311	 77% 19% ..
1	C	311	 80% 17% .
1	D	311	 76% 21% ..
1	E	311	 76% 20% ..
1	F	311	 77% 20% ..

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Mol	Chain	Length	Quality of chain
1	G	311	
1	H	311	
1	I	311	
1	J	311	

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	FUC	B	1	-	-	-	X
2	FUC	B	4	-	-	-	X
2	FUC	C	4	-	-	-	X
2	FUC	C	532	-	-	X	-
2	GAL	C	533	-	-	X	-
2	FUC	C	535	-	-	X	X
2	FUC	D	1	-	-	X	X
2	FUC	D	4	-	-	X	-
2	FUC	E	1	-	-	-	X
2	FUC	E	4	-	-	-	X
2	BGC	E	6	-	-	-	X
2	FUC	F	4	-	-	-	X
2	FUC	G	1	-	-	X	X
2	FUC	G	4	-	-	-	X
2	FUC	J	1	-	-	-	X
2	FUC	J	4	-	-	X	X
2	GAL	J	5	-	-	X	-
2	BGC	J	6	-	-	X	-

2 Entry composition

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.

- Molecule 1 is a protein called Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2403	1517	415	461	10			
1	B	307	Total	C	N	O	S	0	0	0
			2382	1505	407	460	10			
1	C	311	Total	C	N	O	S	0	0	0
			2416	1524	417	465	10			
1	D	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	10			
1	E	309	Total	C	N	O	S	0	0	0
			2406	1518	415	463	10			
1	F	308	Total	C	N	O	S	0	0	0
			2393	1511	411	461	10			
1	G	308	Total	C	N	O	S	0	0	0
			2380	1505	407	458	10			
1	H	300	Total	C	N	O	S	0	0	0
			2291	1456	393	432	10			
1	I	284	Total	C	N	O	S	0	0	0
			2128	1347	371	402	8			
1	J	307	Total	C	N	O	S	0	0	0
			2383	1506	410	457	10			

There are 30 discrepancies between the modelled and reference sequences:

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

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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
E	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
E	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
E	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
H	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
H	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
H	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
I	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
I	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
I	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 a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	6	Total	C	N	O	0	0
			68	38	1	29		
2	C	6	Total	C	N	O	0	0
			68	38	1	29		
2	C	6	Total	C	N	O	0	0
			68	38	1	29		
2	D	6	Total	C	N	O	0	0
			68	38	1	29		
2	E	6	Total	C	N	O	0	0
			68	38	1	29		
2	F	6	Total	C	N	O	0	0
			68	38	1	29		
2	G	6	Total	C	N	O	0	0
			68	38	1	29		
2	J	6	Total	C	N	O	0	0
			68	38	1	29		

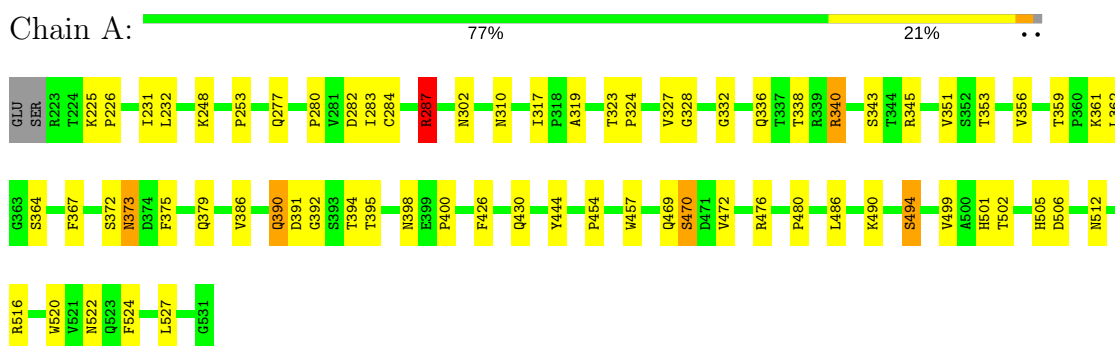
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	54	Total 54	O 54	0	0
3	C	53	Total 53	O 53	0	0
3	D	57	Total 57	O 57	0	0
3	E	46	Total 46	O 46	0	0
3	F	45	Total 45	O 45	0	0
3	G	41	Total 41	O 41	0	0
3	H	36	Total 36	O 36	0	0
3	I	18	Total 18	O 18	0	0
3	J	39	Total 39	O 39	0	0

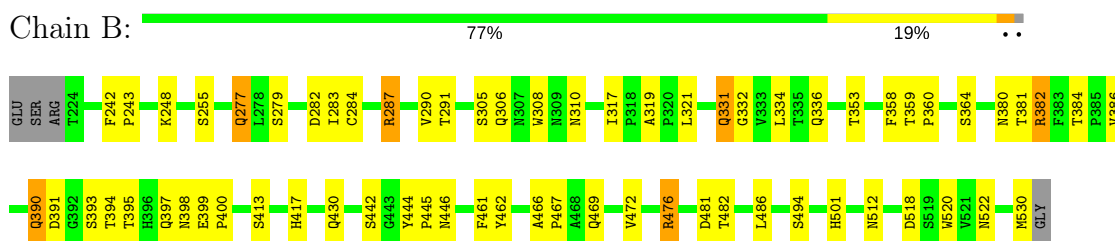
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

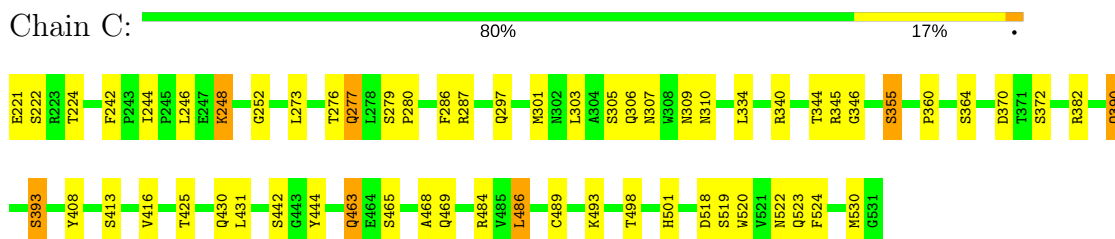
• Molecule 1: Capsid



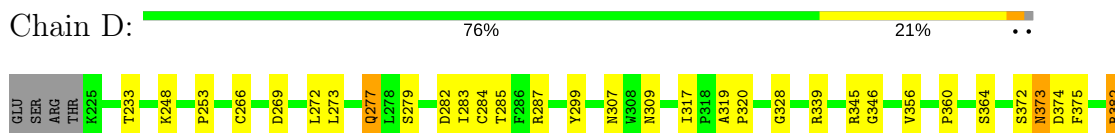
• Molecule 1: Capsid

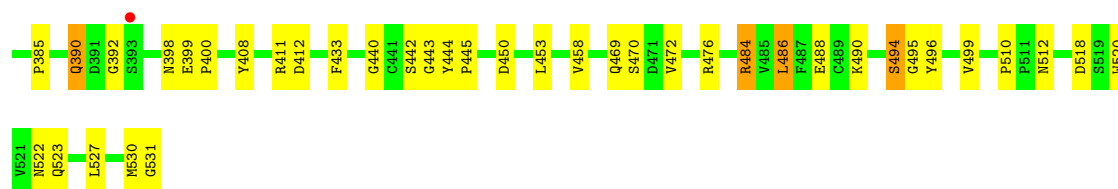


• Molecule 1: Capsid



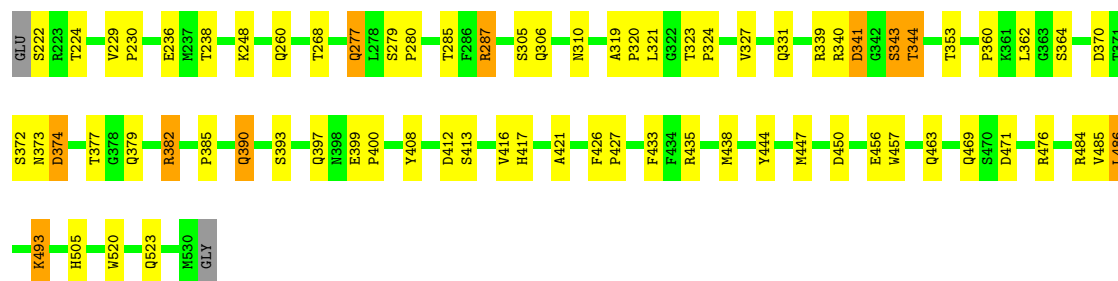
• Molecule 1: Capsid





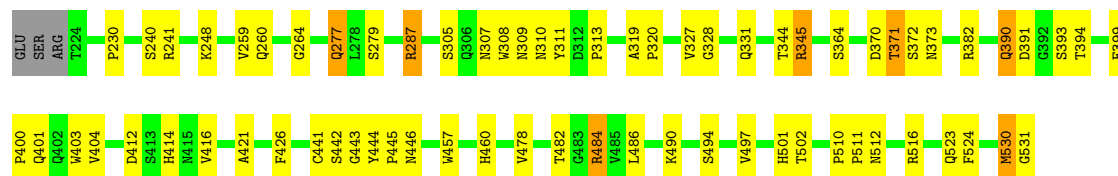
● Molecule 1: Capsid

Chain E: 76% 20% ..



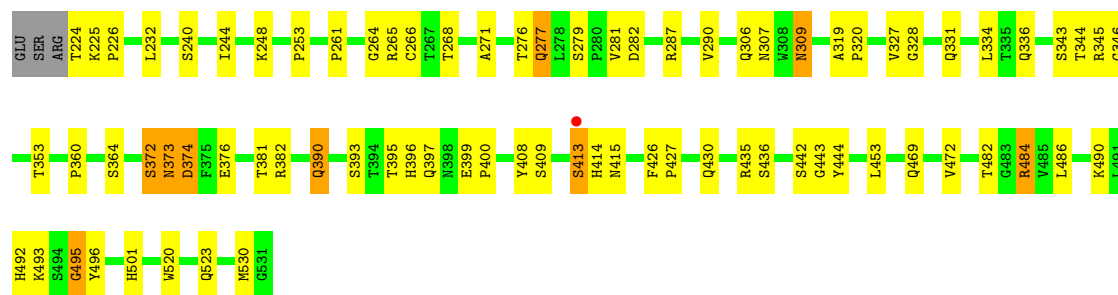
● Molecule 1: Capsid

Chain F: 77% 20% ..



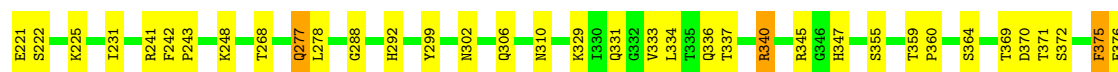
● Molecule 1: Capsid

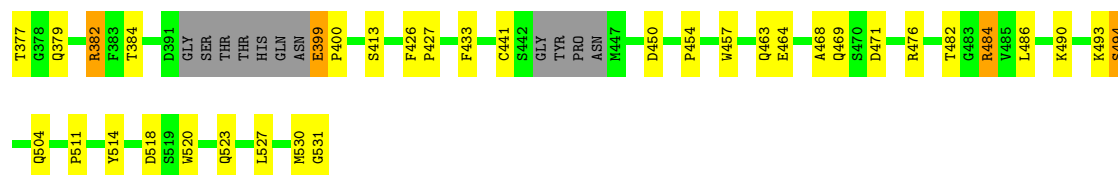
Chain G: 74% 23% ..



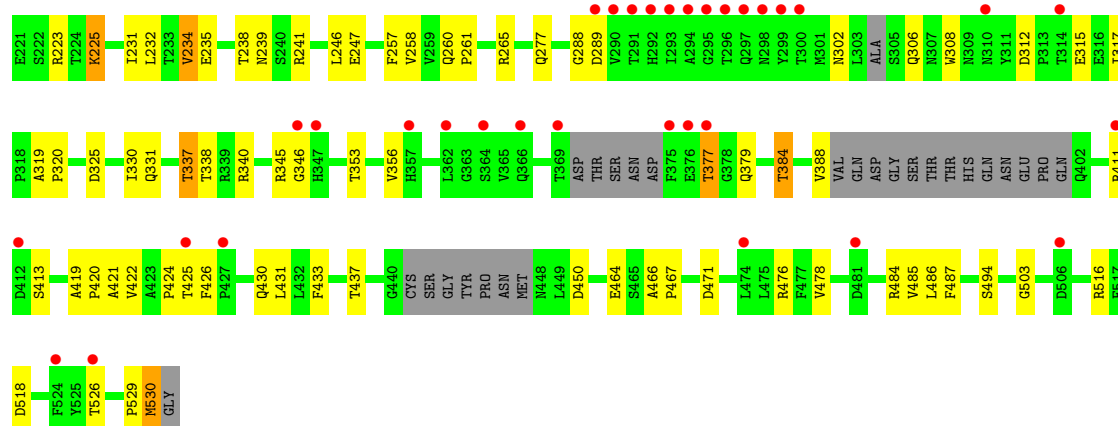
● Molecule 1: Capsid

Chain H: 74% 21% ..

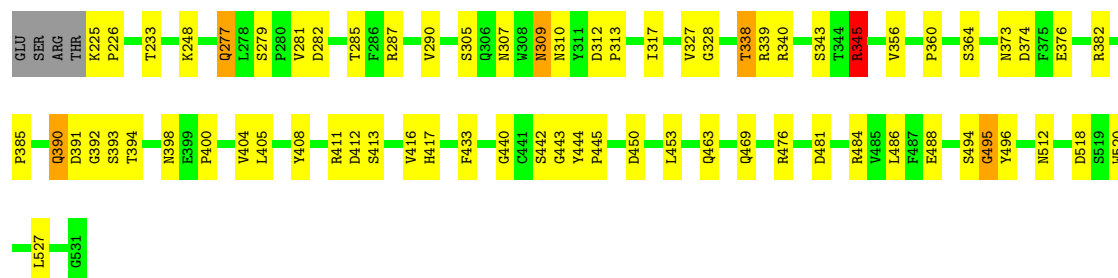
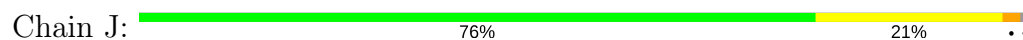




• Molecule 1: Capsid



• Molecule 1: Capsid



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	242.74Å 339.78Å 125.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.04 49.38 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.38-3.04) 99.7 (49.38-3.04)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.223 0.171 , 0.222	Depositor DCC
R_{free} test set	4924 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GAL, NAG, FUC

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	0.90	0/2473	0.89	2/3384 (0.1%)
1	B	0.85	0/2452	0.82	1/3357 (0.0%)
1	C	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	E	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	H	0.80	0/2356	0.85	1/3225 (0.0%)
1	I	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	E	0	1
1	J	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	GLU	CB-CG	5.70	1.62	1.52
1	C	221	GLU	CG-CD	5.38	1.60	1.51
1	C	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	Z	Observed(°)	Ideal(°)
1	I	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	B	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	E	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	A	2403	0	2292	57	0
1	B	2382	0	2264	38	0
1	C	2416	0	2304	42	0
1	D	2386	0	2275	47	0
1	E	2406	0	2297	46	0
1	F	2393	0	2282	56	0
1	G	2380	0	2263	66	0
1	H	2291	0	2167	53	0
1	I	2128	0	1939	49	0
1	J	2383	0	2273	54	0
2	B	68	0	60	2	0
2	C	136	0	120	25	0
2	D	68	0	60	18	0
2	E	68	0	60	6	0
2	F	68	0	60	5	0
2	G	68	0	60	21	0
2	J	68	0	60	20	0
3	A	68	0	0	9	0
3	B	54	0	0	12	0
3	C	53	0	0	13	0
3	D	57	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	46	0	0	13	0
3	F	45	0	0	15	0
3	G	41	0	0	8	0
3	H	36	0	0	16	0
3	I	18	0	0	10	0
3	J	39	0	0	6	0
All	All	24569	0	22836	561	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 561 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)
2:G:1:FUC:O3	1:J:345:ARG:HD3	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	Percentiles	
1	A	307/311 (99%)	293 (95%)	14 (5%)	0	100	100
1	B	305/311 (98%)	294 (96%)	11 (4%)	0	100	100
1	C	309/311 (99%)	294 (95%)	15 (5%)	0	100	100
1	D	305/311 (98%)	297 (97%)	8 (3%)	0	100	100
1	E	307/311 (99%)	290 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	H	294/311 (94%)	278 (95%)	16 (5%)	0	100	100
1	I	274/311 (88%)	252 (92%)	20 (7%)	2 (1%)	25	64
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3018/3110 (97%)	2878 (95%)	138 (5%)	2 (0%)	55	88

All (2) Ramachandran outliers are listed below:

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

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	269/272 (99%)	253 (94%)	16 (6%)	23	58
1	B	268/272 (98%)	247 (92%)	21 (8%)	15	45
1	C	271/272 (100%)	248 (92%)	23 (8%)	12	41
1	D	268/272 (98%)	250 (93%)	18 (7%)	19	53
1	E	271/272 (100%)	248 (92%)	23 (8%)	12	41
1	F	269/272 (99%)	252 (94%)	17 (6%)	21	55
1	G	266/272 (98%)	245 (92%)	21 (8%)	14	44
1	H	249/272 (92%)	228 (92%)	21 (8%)	13	41
1	I	219/272 (80%)	199 (91%)	20 (9%)	11	37
1	J	267/272 (98%)	244 (91%)	23 (9%)	12	40
All	All	2617/2720 (96%)	2414 (92%)	203 (8%)	15	45

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

Mol	Chain	Res	Type
1	E	374	ASP
1	F	416	VAL
1	J	338	THR
1	E	393	SER
1	F	287	ARG

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	E	306	GLN
1	E	505	HIS
1	J	390	GLN
1	E	417	HIS
1	F	297	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 ⓘ

48 carbohydrates 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	FUC	B	1	2	11,11,11	0.56	0	15,16,16	0.70	1 (6%)
2	GAL	B	2	2	11,11,12	0.73	1 (9%)	14,15,17	0.85	0
2	NAG	B	3	2	14,14,15	0.60	0	16,19,21	0.89	1 (6%)
2	FUC	B	4	2	9,10,11	0.44	0	13,14,16	0.82	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	5	2	11,11,12	0.58	0	10,15,17	0.83	1 (10%)
2	BGC	B	6	2	11,11,12	0.55	0	15,15,17	0.91	1 (6%)
2	FUC	C	1	2	11,11,11	1.79	3 (27%)	15,16,16	3.82	6 (40%)
2	GAL	C	2	2	11,11,12	2.04	5 (45%)	14,15,17	1.87	4 (28%)
2	NAG	C	3	2	14,14,15	1.05	1 (7%)	16,19,21	1.68	3 (18%)
2	FUC	C	4	2	9,10,11	1.57	2 (22%)	13,14,16	3.06	6 (46%)
2	GAL	C	5	2	11,11,12	0.57	0	10,15,17	1.35	1 (10%)
2	FUC	C	532	2	11,11,11	1.26	1 (9%)	15,16,16	3.28	5 (33%)
2	GAL	C	533	2	11,11,12	1.51	2 (18%)	14,15,17	2.32	7 (50%)
2	NAG	C	534	2	14,14,15	0.99	0	16,19,21	1.68	3 (18%)
2	FUC	C	535	2	9,10,11	0.43	0	13,14,16	0.85	1 (7%)
2	GAL	C	536	2	11,11,12	0.57	0	10,15,17	0.82	1 (10%)
2	BGC	C	537	2	11,11,12	0.55	0	15,15,17	0.99	1 (6%)
2	BGC	C	6	2	11,11,12	0.55	0	15,15,17	1.88	4 (26%)
2	FUC	D	1	2	11,11,11	0.58	0	15,16,16	0.63	0
2	GAL	D	2	2	11,11,12	2.03	6 (54%)	14,15,17	3.48	5 (35%)
2	NAG	D	3	2	14,14,15	1.30	1 (7%)	16,19,21	1.54	3 (18%)
2	FUC	D	4	2	9,10,11	0.50	0	13,14,16	0.96	1 (7%)
2	GAL	D	5	2	11,11,12	0.85	0	10,15,17	1.55	2 (20%)
2	BGC	D	6	2	11,11,12	1.19	1 (9%)	15,15,17	2.69	6 (40%)
2	FUC	E	1	2	11,11,11	0.75	0	15,16,16	0.91	1 (6%)
2	GAL	E	2	2	11,11,12	2.04	4 (36%)	14,15,17	2.07	5 (35%)
2	NAG	E	3	2	14,14,15	0.98	1 (7%)	16,19,21	1.40	2 (12%)
2	FUC	E	4	2	9,10,11	0.42	0	13,14,16	0.82	1 (7%)
2	GAL	E	5	2	11,11,12	1.21	2 (18%)	10,15,17	1.98	4 (40%)
2	BGC	E	6	2	11,11,12	1.26	1 (9%)	15,15,17	2.47	6 (40%)
2	FUC	F	1	2	11,11,11	0.55	0	15,16,16	0.70	1 (6%)
2	GAL	F	2	2	11,11,12	0.72	1 (9%)	14,15,17	0.86	0
2	NAG	F	3	2	14,14,15	0.59	0	16,19,21	0.88	1 (6%)
2	FUC	F	4	2	9,10,11	0.45	0	13,14,16	0.82	1 (7%)
2	GAL	F	5	2	11,11,12	0.58	0	10,15,17	0.83	1 (10%)
2	BGC	F	6	2	11,11,12	0.56	0	15,15,17	0.94	1 (6%)
2	FUC	G	1	2	11,11,11	0.54	0	15,16,16	0.70	1 (6%)
2	GAL	G	2	2	11,11,12	0.72	1 (9%)	14,15,17	0.85	0
2	NAG	G	3	2	14,14,15	0.59	0	16,19,21	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	G	4	2	9,10,11	0.43	0	13,14,16	0.82	0
2	GAL	G	5	2	11,11,12	0.58	0	10,15,17	0.84	1 (10%)
2	BGC	G	6	2	11,11,12	0.56	0	15,15,17	0.91	1 (6%)
2	FUC	J	1	2	11,11,11	0.55	0	15,16,16	0.71	1 (6%)
2	GAL	J	2	2	11,11,12	0.73	1 (9%)	14,15,17	0.86	0
2	NAG	J	3	2	14,14,15	0.59	0	16,19,21	0.87	1 (6%)
2	FUC	J	4	2	9,10,11	0.44	0	13,14,16	0.82	0
2	GAL	J	5	2	11,11,12	0.58	0	10,15,17	0.84	1 (10%)
2	BGC	J	6	2	11,11,12	0.55	0	15,15,17	0.92	1 (6%)

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	FUC	B	1	2	-	0/0/20/20	0/1/1/1
2	GAL	B	2	2	-	0/2/18/22	0/1/1/1
2	NAG	B	3	2	-	0/6/22/26	0/1/1/1
2	FUC	B	4	2	-	0/0/17/20	0/1/1/1
2	GAL	B	5	2	-	0/2/18/22	0/1/1/1
2	BGC	B	6	2	-	0/2/18/22	0/1/1/1
2	FUC	C	1	2	-	0/0/20/20	0/1/1/1
2	GAL	C	2	2	-	0/2/18/22	0/1/1/1
2	NAG	C	3	2	-	0/6/22/26	0/1/1/1
2	FUC	C	4	2	-	0/0/17/20	0/1/1/1
2	GAL	C	5	2	-	0/2/18/22	0/1/1/1
2	FUC	C	532	2	-	0/0/20/20	0/1/1/1
2	GAL	C	533	2	-	0/2/18/22	0/1/1/1
2	NAG	C	534	2	-	0/6/22/26	0/1/1/1
2	FUC	C	535	2	-	0/0/17/20	0/1/1/1
2	GAL	C	536	2	-	0/2/18/22	0/1/1/1
2	BGC	C	537	2	-	0/2/18/22	0/1/1/1
2	BGC	C	6	2	-	0/2/18/22	0/1/1/1
2	FUC	D	1	2	-	0/0/20/20	0/1/1/1
2	GAL	D	2	2	-	0/2/18/22	0/1/1/1
2	NAG	D	3	2	-	0/6/22/26	0/1/1/1
2	FUC	D	4	2	-	0/0/17/20	0/1/1/1
2	GAL	D	5	2	-	0/2/18/22	0/1/1/1
2	BGC	D	6	2	-	0/2/18/22	0/1/1/1
2	FUC	E	1	2	-	0/0/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	E	2	2	-	0/2/18/22	0/1/1/1
2	NAG	E	3	2	-	0/6/22/26	0/1/1/1
2	FUC	E	4	2	-	0/0/17/20	0/1/1/1
2	GAL	E	5	2	-	0/2/18/22	0/1/1/1
2	BGC	E	6	2	-	0/2/18/22	0/1/1/1
2	FUC	F	1	2	-	0/0/20/20	0/1/1/1
2	GAL	F	2	2	-	0/2/18/22	0/1/1/1
2	NAG	F	3	2	-	0/6/22/26	0/1/1/1
2	FUC	F	4	2	-	0/0/17/20	0/1/1/1
2	GAL	F	5	2	-	0/2/18/22	0/1/1/1
2	BGC	F	6	2	-	0/2/18/22	0/1/1/1
2	FUC	G	1	2	-	0/0/20/20	0/1/1/1
2	GAL	G	2	2	-	0/2/18/22	0/1/1/1
2	NAG	G	3	2	-	0/6/22/26	0/1/1/1
2	FUC	G	4	2	-	0/0/17/20	0/1/1/1
2	GAL	G	5	2	-	0/2/18/22	0/1/1/1
2	BGC	G	6	2	-	0/2/18/22	0/1/1/1
2	FUC	J	1	2	-	0/0/20/20	0/1/1/1
2	GAL	J	2	2	-	0/2/18/22	0/1/1/1
2	NAG	J	3	2	-	0/6/22/26	0/1/1/1
2	FUC	J	4	2	-	0/0/17/20	0/1/1/1
2	GAL	J	5	2	-	0/2/18/22	0/1/1/1
2	BGC	J	6	2	-	0/2/18/22	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	GAL	O5-C1	-4.02	1.36	1.44
2	C	1	FUC	O5-C5	-3.83	1.35	1.44
2	D	3	NAG	C3-C4	-3.75	1.46	1.52
2	E	2	GAL	O5-C5	-3.74	1.35	1.44
2	C	533	GAL	O5-C1	-3.51	1.37	1.44

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	O5-C1-C2	-10.66	102.95	110.77
2	C	1	FUC	C6-C5-C4	-10.19	94.92	113.07
2	C	532	FUC	O5-C1-C2	-9.38	94.48	110.04
2	C	1	FUC	O5-C5-C4	-7.75	96.85	109.62
2	C	4	FUC	C6-C5-C4	-6.83	100.90	113.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

40 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GAL	1	0
2	B	3	NAG	1	0
2	B	4	FUC	2	0
2	C	1	FUC	2	0
2	C	2	GAL	2	0
2	C	3	NAG	2	0
2	C	4	FUC	4	0
2	C	5	GAL	3	0
2	C	532	FUC	8	0
2	C	533	GAL	6	0
2	C	534	NAG	2	0
2	C	535	FUC	8	0
2	C	536	GAL	3	0
2	C	537	BGC	3	0
2	C	6	BGC	3	0
2	D	1	FUC	9	0
2	D	2	GAL	3	0
2	D	3	NAG	3	0
2	D	4	FUC	12	0
2	D	5	GAL	2	0
2	D	6	BGC	2	0
2	E	2	GAL	1	0
2	E	3	NAG	1	0
2	E	4	FUC	2	0
2	E	5	GAL	1	0
2	E	6	BGC	4	0
2	F	2	GAL	4	0
2	F	4	FUC	3	0
2	F	6	BGC	1	0
2	G	1	FUC	13	0
2	G	2	GAL	4	0
2	G	3	NAG	1	0
2	G	4	FUC	4	0
2	G	5	GAL	4	0
2	G	6	BGC	3	0
2	J	1	FUC	5	0
2	J	2	GAL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	4	FUC	13	0
2	J	5	GAL	6	0
2	J	6	BGC	6	0

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, 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	309/311 (99%)	-0.74	0 100 100	10, 22, 54, 90	0
1	B	307/311 (98%)	-0.73	0 100 100	15, 26, 51, 65	0
1	C	311/311 (100%)	-0.57	0 100 100	13, 27, 49, 64	0
1	D	307/311 (98%)	-0.59	1 (0%) 93 82	11, 27, 59, 82	0
1	E	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%) 93 82	22, 38, 63, 104	0
1	H	300/311 (96%)	-0.33	0 100 100	17, 41, 79, 109	0
1	I	284/311 (91%)	0.87	33 (11%) 5 2	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%)	-0.45	35 (1%) 80 55	10, 33, 83, 140	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	296	THR	4.2
1	I	300	THR	3.8
1	I	411	ARG	3.2
1	I	297	GLN	3.2
1	I	293	ILE	3.1

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	FUC	F	4	10/11	0.70	0.49	13.53	119,120,121,121	0
2	BGC	E	6	11/12	0.72	0.61	13.04	108,109,109,109	0
2	FUC	J	4	10/11	0.75	0.49	6.07	107,108,109,109	0
2	FUC	C	4	10/11	0.77	0.30	4.34	92,96,97,98	0
2	FUC	B	4	10/11	0.78	0.34	4.06	99,100,101,101	0
2	FUC	G	4	10/11	0.78	0.37	3.42	100,101,102,102	0
2	FUC	B	1	11/11	0.82	0.28	3.33	74,77,80,84	0
2	FUC	G	1	11/11	0.79	0.25	3.07	70,74,79,85	0
2	FUC	E	4	10/11	0.86	0.32	2.92	73,75,76,77	0
2	FUC	C	535	10/11	0.69	0.40	2.64	91,93,94,95	0
2	FUC	E	1	11/11	0.87	0.23	2.49	57,61,63,68	0
2	FUC	D	1	11/11	0.81	0.30	2.47	84,87,89,92	0
2	FUC	J	1	11/11	0.83	0.29	2.11	83,84,88,92	0
2	FUC	D	4	10/11	0.74	0.38	1.53	97,99,99,99	0
2	FUC	F	1	11/11	0.87	0.28	1.38	100,101,104,108	0
2	FUC	C	532	11/11	0.86	0.28	1.24	73,74,79,83	0
2	FUC	C	1	11/11	0.86	0.20	1.21	71,72,78,85	0
2	GAL	B	5	11/12	0.68	0.49	-	118,119,123,126	0
2	GAL	C	533	11/12	0.76	0.34	-	85,88,90,93	0
2	GAL	J	5	11/12	0.74	0.49	-	122,123,126,129	0
2	GAL	D	2	11/12	0.78	0.38	-	92,94,96,100	0
2	NAG	E	3	14/15	0.81	0.43	-	81,83,88,93	0
2	NAG	B	3	14/15	0.82	0.45	-	101,104,108,113	0
2	BGC	B	6	11/12	0.54	0.60	-	129,130,130,131	0
2	NAG	D	3	14/15	0.83	0.40	-	97,102,106,111	0
2	GAL	F	2	11/12	0.76	0.41	-	111,112,114,117	0
2	BGC	F	6	11/12	0.72	0.41	-	134,136,136,136	0
2	NAG	F	3	14/15	0.84	0.39	-	120,121,124,126	0
2	GAL	E	2	11/12	0.86	0.32	-	71,73,75,79	0
2	GAL	E	5	11/12	0.75	0.63	-	96,98,101,105	0
2	NAG	J	3	14/15	0.80	0.46	-	109,111,114,119	0
2	GAL	C	5	11/12	0.58	0.51	-	115,117,120,124	0
2	GAL	B	2	11/12	0.87	0.35	-	88,91,92,98	0
2	NAG	G	3	14/15	0.68	0.34	-	97,103,106,110	0
2	BGC	G	6	11/12	0.62	0.62	-	113,116,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BGC	C	6	11/12	0.47	0.76	-	128,130,130,130	0
2	BGC	C	537	11/12	0.69	0.56	-	123,125,126,126	0
2	GAL	C	2	11/12	0.85	0.32	-	89,92,93,98	0
2	NAG	C	3	14/15	0.80	0.38	-	99,103,106,111	0
2	NAG	C	534	14/15	0.81	0.37	-	94,97,103,108	0
2	GAL	G	2	11/12	0.83	0.27	-	93,96,97,99	0
2	GAL	G	5	11/12	0.67	0.40	-	112,113,114,116	0
2	GAL	D	5	11/12	0.64	0.49	-	114,116,120,123	0
2	BGC	D	6	11/12	0.80	0.55	-	124,126,126,127	0
2	GAL	C	536	11/12	0.59	0.58	-	113,115,118,122	0
2	BGC	J	6	11/12	0.64	0.67	-	132,133,133,133	0
2	GAL	J	2	11/12	0.83	0.31	-	95,96,99,104	0
2	GAL	F	5	11/12	0.70	0.31	-	128,130,132,134	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.