



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:01 PM 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 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
<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:

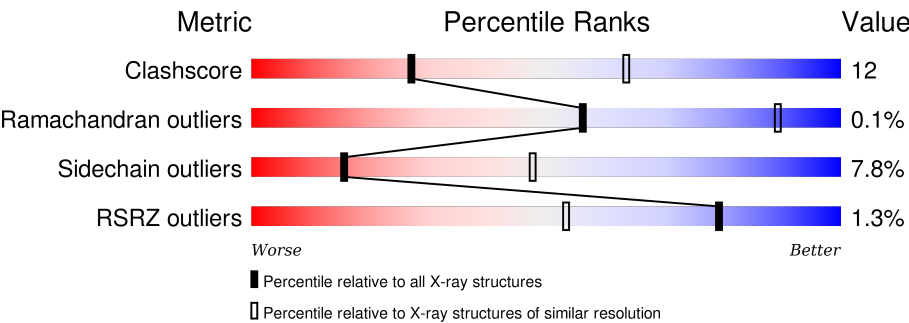
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

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))
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (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	<div><div></div><div>77%21%..</div></div>
1	B	311	<div><div></div><div>77%19%..</div></div>
1	C	311	<div><div></div><div>80%17%. </div></div>
1	D	311	<div><div></div><div>76%21%..</div></div>
1	E	311	<div><div>%</div><div>76%20%..</div></div>
1	F	311	<div><div></div><div>77%20%..</div></div>
1	G	311	<div><div></div><div>74%23%. </div></div>

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Mol	Chain	Length	Quality of chain
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		

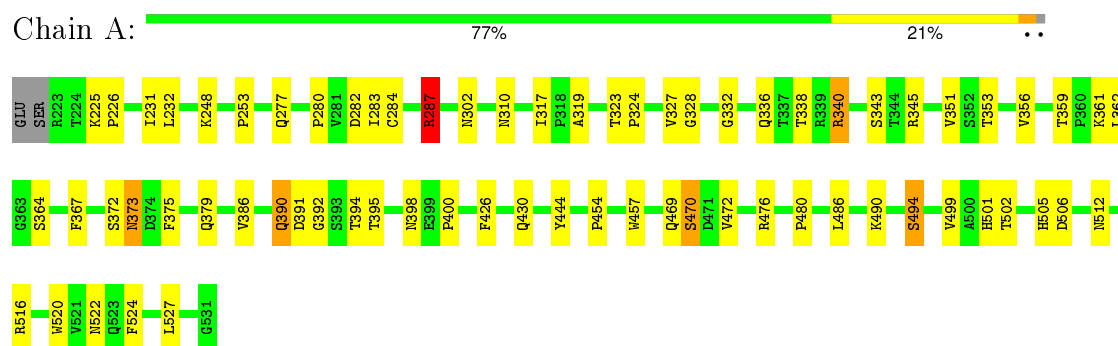
- Molecule 3 is water.

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

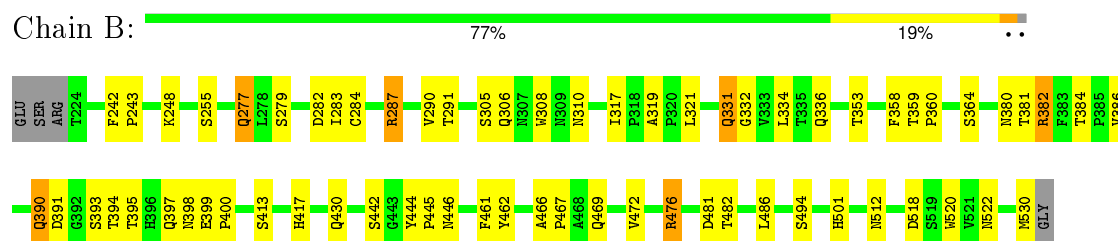
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

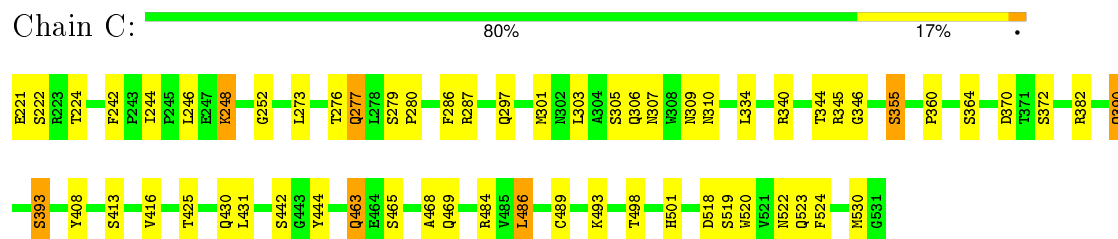
• Molecule 1: Capsid



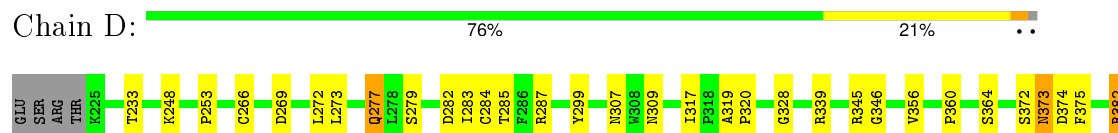
• Molecule 1: Capsid

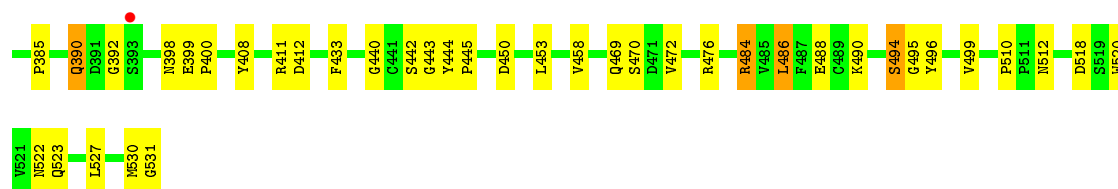


• Molecule 1: Capsid

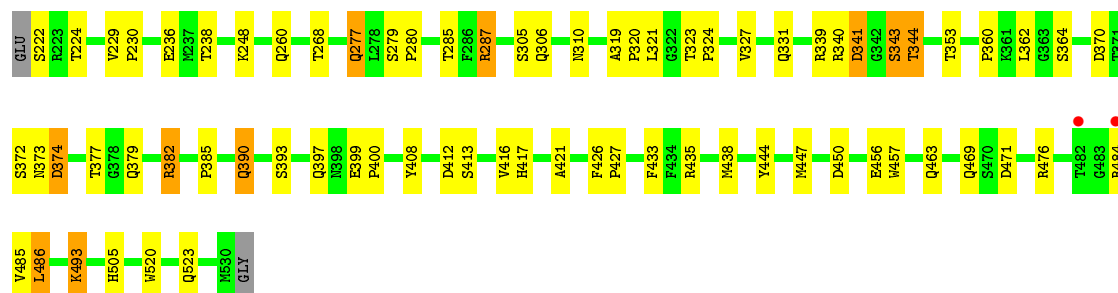
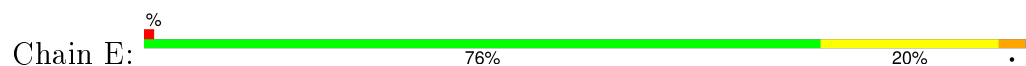


• Molecule 1: Capsid

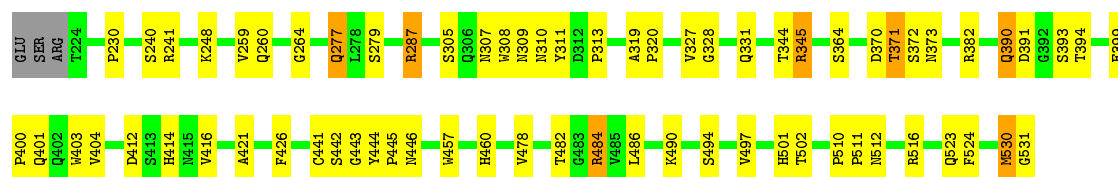
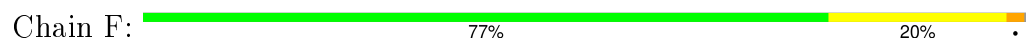




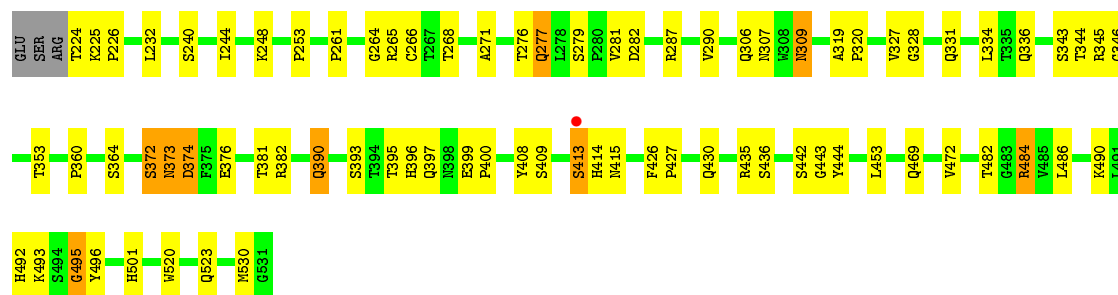
• Molecule 1: Capsid



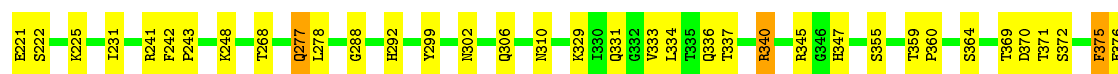
• Molecule 1: Capsid

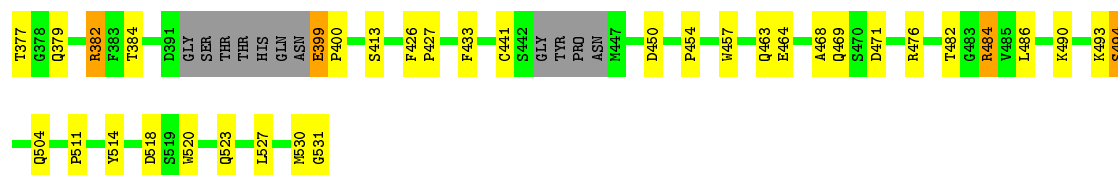


• Molecule 1: Capsid

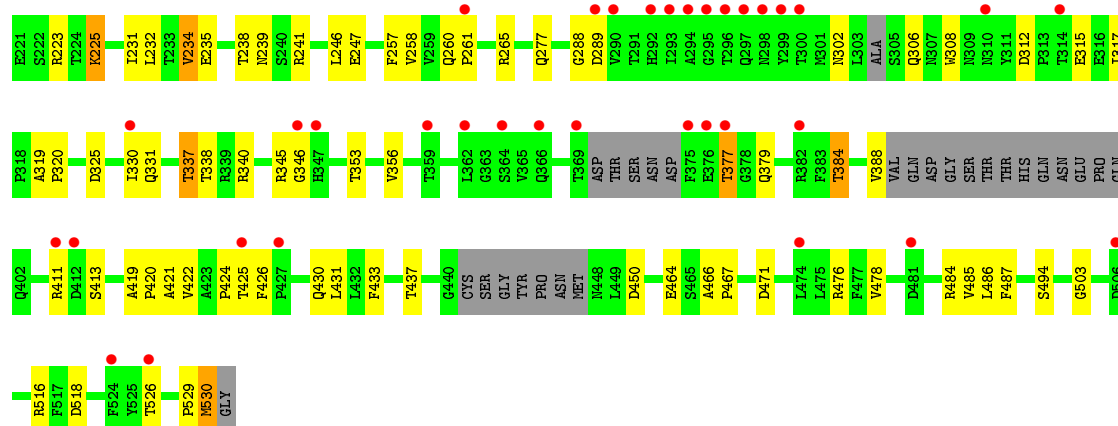


• Molecule 1: Capsid

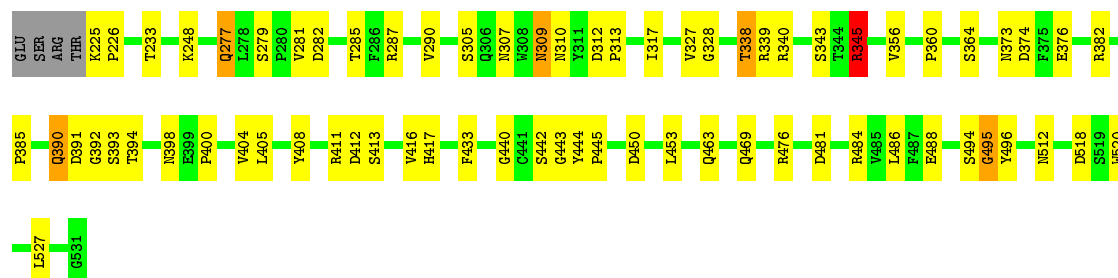




• Molecule 1: Capsid



• 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 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	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 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 98969 reflections	Xtriage
F_o, F_c correlation	0.92	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, 0.375 respectively for untwinned datasets, and 0.333, 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

All (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
1	I	232	LEU	CA-CB-CG	6.38	129.98	115.30
1	E	486	LEU	CA-CB-CG	-6.18	101.09	115.30
1	D	382	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	225	LYS	CD-CE-NZ	-5.84	98.26	111.70
1	D	269	ASP	CB-CG-OD1	5.71	123.43	118.30
1	G	374	ASP	N-CA-C	5.65	126.25	111.00
1	A	287	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	J	496	TYR	N-CA-CB	-5.58	100.55	110.60
1	H	241	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	F	241	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	496	TYR	N-CA-CB	-5.38	100.91	110.60
1	C	486	LEU	CA-CB-CG	-5.25	103.23	115.30
1	E	374	ASP	N-CA-C	5.06	124.67	111.00
1	D	269	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	463	GLN	CB-CA-C	-5.01	100.37	110.40

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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:H:376:GLU:HA	3:H:149:HOH:O	1.48	1.12
2:G:5:GAL:H1	2:G:6:BGC:H6C1	1.11	1.10
1:J:394:THR:HB	1:J:398:ASN:HD21	1.04	1.09
2:G:5:GAL:C1	2:G:6:BGC:H6C1	1.82	1.08
2:D:1:FUC:H61	2:D:4:FUC:H61	1.37	1.07
1:J:226:PRO:HD2	3:J:541:HOH:O	1.52	1.06
2:C:532:FUC:H61	2:C:535:FUC:H61	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:FUC:H5	2:C:2:GAL:O1	1.57	1.05
1:G:409:SER:HB2	1:G:413:SER:CB	1.87	1.04
1:E:417:HIS:HD2	3:E:148:HOH:O	1.37	1.04
2:J:1:FUC:H61	2:J:4:FUC:H61	1.08	1.03
2:J:5:GAL:O5	2:J:6:BGC:H3	1.59	1.02
1:E:310:ASN:HB2	3:E:155:HOH:O	1.59	1.02
2:C:532:FUC:H5	2:C:533:GAL:O1	1.61	1.01
1:H:345:ARG:HA	3:H:542:HOH:O	1.59	1.00
2:C:3:NAG:H61	2:C:4:FUC:C1	1.92	1.00
1:G:409:SER:HB2	1:G:413:SER:HB3	1.40	1.00
1:J:394:THR:HB	1:J:398:ASN:ND2	1.75	0.99
2:J:1:FUC:C6	2:J:4:FUC:H61	1.92	0.99
1:F:370:ASP:HB2	3:F:119:HOH:O	1.62	0.99
2:F:2:GAL:O1	2:F:4:FUC:H5	1.65	0.97
1:F:523:GLN:HB2	3:F:187:HOH:O	1.69	0.93
1:A:336:GLN:OE1	1:A:375:PHE:HD1	1.50	0.93
1:D:307:ASN:HA	3:D:553:HOH:O	1.67	0.93
1:J:345:ARG:HH21	1:J:345:ARG:CG	1.82	0.92
1:A:336:GLN:HE21	1:A:379:GLN:HB2	1.33	0.92
1:C:370:ASP:HB2	3:C:547:HOH:O	1.69	0.91
2:D:1:FUC:C6	2:D:4:FUC:H61	2.00	0.91
1:I:337:THR:HG21	3:J:539:HOH:O	1.69	0.91
1:J:345:ARG:HG2	1:J:345:ARG:NH2	1.84	0.89
2:F:6:BGC:H6C1	3:F:533:HOH:O	1.72	0.88
2:C:534:NAG:H61	2:C:535:FUC:C1	2.03	0.88
1:A:390:GLN:OE1	1:A:391:ASP:O	1.91	0.87
1:F:494:SER:HB2	3:F:551:HOH:O	1.74	0.87
2:J:2:GAL:O1	2:J:4:FUC:H5	1.74	0.86
1:E:370:ASP:HB2	3:E:44:HOH:O	1.74	0.86
2:J:1:FUC:H61	2:J:4:FUC:C6	2.00	0.86
1:H:531:GLY:HA2	3:H:544:HOH:O	1.75	0.85
2:G:5:GAL:H1	2:G:6:BGC:C6	2.02	0.85
1:B:291:THR:HG21	3:B:563:HOH:O	1.75	0.85
2:D:3:NAG:H61	2:D:4:FUC:C1	2.07	0.83
2:G:1:FUC:O3	1:J:345:ARG:CD	2.25	0.83
1:G:453:LEU:HD21	1:G:495:GLY:O	1.78	0.83
1:D:442:SER:HA	1:F:344:THR:O	1.79	0.83
1:D:518:ASP:HB3	3:D:558:HOH:O	1.80	0.82
1:A:394:THR:HB	1:A:398:ASN:HD21	1.43	0.82
1:E:484:ARG:HB3	3:E:556:HOH:O	1.78	0.82
1:F:390:GLN:HG2	1:F:444:TYR:C	2.01	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:HB2	3:B:48:HOH:O	1.80	0.81
1:A:391:ASP:OD2	1:A:394:THR:HG23	1.82	0.79
1:G:373:ASN:ND2	1:G:373:ASN:N	2.30	0.79
2:C:536:GAL:C1	2:C:537:BGC:O6	2.31	0.79
1:E:523:GLN:HB2	3:E:553:HOH:O	1.82	0.79
1:J:338:THR:CG2	1:J:345:ARG:NH1	2.46	0.79
1:I:337:THR:CG2	1:I:338:THR:OG1	2.30	0.79
2:E:3:NAG:H61	2:E:4:FUC:C1	2.13	0.78
1:F:382:ARG:HD2	3:F:175:HOH:O	1.83	0.78
2:J:5:GAL:O5	2:J:6:BGC:H5	1.83	0.78
1:C:469:GLN:HG3	1:C:520:TRP:CD1	2.19	0.78
1:D:453:LEU:HD21	1:D:495:GLY:O	1.83	0.78
1:G:382:ARG:HD2	3:G:189:HOH:O	1.84	0.77
1:D:317:ILE:HG22	1:H:340:ARG:HD3	1.64	0.77
1:F:530:MET:HA	3:F:130:HOH:O	1.83	0.76
1:D:307:ASN:OD1	1:D:309:ASN:HB2	1.84	0.76
2:E:6:BGC:O1	2:E:6:BGC:C6	2.30	0.76
1:J:338:THR:HG22	1:J:345:ARG:NH1	2.01	0.75
1:I:356:VAL:CG1	1:I:411:ARG:HD2	2.15	0.75
1:A:336:GLN:OE1	1:A:375:PHE:CD1	2.39	0.75
2:G:2:GAL:O5	2:G:4:FUC:H5	1.87	0.75
1:J:307:ASN:ND2	1:J:309:ASN:HB2	2.02	0.75
1:I:356:VAL:HG12	1:I:411:ARG:HD2	1.67	0.75
1:I:337:THR:HG23	1:I:338:THR:OG1	1.87	0.74
1:F:310:ASN:HA	3:F:546:HOH:O	1.86	0.74
1:A:494:SER:HB2	3:A:58:HOH:O	1.85	0.74
2:D:3:NAG:C6	2:D:4:FUC:C1	2.65	0.74
1:B:476:ARG:HD3	1:B:518:ASP:OD2	1.88	0.74
2:D:1:FUC:H61	2:D:4:FUC:C6	2.17	0.73
1:C:430:GLN:HG3	1:C:501:HIS:O	1.88	0.73
1:C:425:THR:HA	3:C:551:HOH:O	1.87	0.73
1:C:393:SER:OG	2:C:4:FUC:H2	1.88	0.73
2:C:533:GAL:O5	2:C:535:FUC:H5	1.88	0.73
1:B:469:GLN:HB2	1:B:520:TRP:CG	2.23	0.73
1:I:485:VAL:HG23	3:I:541:HOH:O	1.89	0.72
2:D:2:GAL:O5	2:D:4:FUC:H5	1.88	0.72
1:J:391:ASP:HB3	1:J:394:THR:OG1	1.89	0.72
1:H:379:GLN:HB3	3:H:185:HOH:O	1.90	0.71
1:G:409:SER:HB2	1:G:413:SER:HB2	1.72	0.71
1:J:394:THR:CB	1:J:398:ASN:HD21	1.93	0.71
1:J:453:LEU:HD21	1:J:495:GLY:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:469:GLN:HG3	1:J:520:TRP:CD1	2.25	0.71
1:G:390:GLN:HG3	1:G:444:TYR:H	1.56	0.70
1:H:268:THR:HG23	1:H:493:LYS:HA	1.71	0.70
2:C:532:FUC:H5	2:C:533:GAL:C2	2.20	0.70
1:D:494:SER:HB2	3:D:136:HOH:O	1.91	0.70
1:I:476:ARG:HD3	1:I:518:ASP:OD2	1.91	0.70
1:D:440:GLY:HA3	1:F:344:THR:HG21	1.74	0.70
1:C:277:GLN:HG3	1:C:306:GLN:HE22	1.56	0.70
2:B:3:NAG:O6	2:B:4:FUC:C1	2.40	0.69
1:I:430:GLN:HE22	1:I:503:GLY:H	1.39	0.69
1:I:337:THR:HG22	1:I:338:THR:CB	2.22	0.69
1:J:310:ASN:HA	3:J:534:HOH:O	1.92	0.69
1:B:310:ASN:HB3	3:B:213:HOH:O	1.92	0.68
1:J:307:ASN:HD21	1:J:309:ASN:HB2	1.58	0.68
1:H:347:HIS:HD2	1:H:372:SER:CB	2.07	0.68
1:B:390:GLN:HG2	1:B:444:TYR:C	2.14	0.68
1:A:391:ASP:HB3	1:A:394:THR:HG23	1.76	0.68
1:G:443:GLY:HA2	2:G:1:FUC:H61	1.77	0.67
1:I:239:ASN:N	1:I:246:LEU:HG	2.09	0.67
1:E:360:PRO:HD2	1:E:408:TYR:O	1.94	0.67
1:A:340:ARG:HG2	3:B:45:HOH:O	1.93	0.67
1:E:236:GLU:HA	3:E:533:HOH:O	1.93	0.67
1:J:390:GLN:HG2	1:J:444:TYR:C	2.14	0.67
1:A:231:ILE:O	1:A:231:ILE:HG22	1.94	0.67
1:A:336:GLN:NE2	1:A:379:GLN:HB2	2.09	0.67
1:A:394:THR:CB	1:A:398:ASN:HD21	2.08	0.67
1:J:277:GLN:OE1	1:J:279:SER:HB3	1.95	0.67
1:H:336:GLN:HE21	1:H:375:PHE:HD1	1.43	0.66
2:C:532:FUC:H5	2:C:533:GAL:C1	2.25	0.66
1:G:409:SER:CB	1:G:413:SER:CB	2.71	0.66
1:D:442:SER:OG	2:D:1:FUC:H1	1.96	0.66
1:G:482:THR:OG1	1:G:484:ARG:HG2	1.94	0.66
2:J:2:GAL:C1	2:J:4:FUC:H5	2.26	0.66
1:B:331:GLN:HG3	3:B:560:HOH:O	1.96	0.66
1:A:356:VAL:HG13	3:A:22:HOH:O	1.95	0.66
1:G:443:GLY:H	2:G:1:FUC:C6	2.09	0.65
2:C:5:GAL:C1	2:C:6:BGC:O6	2.44	0.65
1:A:470:SER:HB3	1:A:520:TRP:HB3	1.77	0.65
1:J:345:ARG:HD2	1:J:374:ASP:OD1	1.97	0.65
2:D:1:FUC:C5	2:D:4:FUC:H61	2.27	0.65
1:A:373:ASN:N	1:A:373:ASN:OD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:GAL:H1	2:C:6:BGC:O6	1.97	0.65
1:I:238:THR:O	1:I:246:LEU:HD11	1.97	0.65
1:A:302:ASN:HB3	3:A:536:HOH:O	1.97	0.64
2:G:2:GAL:O1	2:G:4:FUC:H5	1.96	0.64
1:I:345:ARG:CB	3:I:542:HOH:O	2.46	0.64
2:J:5:GAL:H2	2:J:6:BGC:H6C1	1.80	0.64
1:B:242:PHE:CD2	1:B:243:PRO:HD2	2.32	0.64
1:G:469:GLN:HG3	1:G:520:TRP:CD1	2.33	0.64
1:D:373:ASN:N	1:D:373:ASN:OD1	2.29	0.64
1:I:337:THR:HG22	1:I:338:THR:HB	1.79	0.64
1:H:399:GLU:HB2	1:H:400:PRO:HA	1.79	0.64
1:I:319:ALA:HB1	1:I:320:PRO:HD2	1.78	0.64
1:G:453:LEU:CD2	1:G:495:GLY:O	2.46	0.64
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.33	0.64
1:G:277:GLN:OE1	1:G:279:SER:HB3	1.97	0.64
1:J:476:ARG:HD3	1:J:518:ASP:OD2	1.98	0.64
1:E:390:GLN:HG3	1:E:444:TYR:H	1.63	0.64
1:E:373:ASN:OD1	1:E:373:ASN:N	2.30	0.63
1:A:391:ASP:HB3	1:A:394:THR:CG2	2.28	0.63
1:H:221:GLU:N	1:H:469:GLN:NE2	2.46	0.63
1:I:225:LYS:NZ	1:I:464:GLU:O	2.24	0.63
1:G:469:GLN:HB2	1:G:520:TRP:CG	2.33	0.63
1:F:482:THR:OG1	1:F:484:ARG:HG2	1.99	0.63
1:G:443:GLY:HA2	2:G:1:FUC:C6	2.29	0.63
2:B:2:GAL:O5	2:B:4:FUC:H5	1.97	0.63
1:H:426:PHE:CD2	1:H:427:PRO:HD2	2.33	0.63
1:F:287:ARG:HD3	3:F:532:HOH:O	1.98	0.62
3:B:68:HOH:O	1:E:382:ARG:HD2	1.99	0.62
1:J:373:ASN:N	1:J:373:ASN:OD1	2.30	0.62
2:C:532:FUC:H61	2:C:535:FUC:C6	2.22	0.62
2:J:5:GAL:O5	2:J:6:BGC:C3	2.30	0.62
1:D:392:GLY:HA3	2:D:4:FUC:O5	2.00	0.62
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.81	0.62
1:F:531:GLY:HA2	3:F:141:HOH:O	1.98	0.62
1:I:317:ILE:HD12	1:I:319:ALA:O	2.00	0.62
1:H:463:GLN:HG2	3:H:547:HOH:O	1.98	0.62
2:D:1:FUC:O3	1:F:345:ARG:HG3	2.00	0.61
2:G:2:GAL:C1	2:G:4:FUC:H5	2.30	0.61
2:C:536:GAL:H1	2:C:537:BGC:O6	1.99	0.61
1:D:531:GLY:HA3	3:D:113:HOH:O	1.99	0.61
2:D:1:FUC:O5	2:D:4:FUC:H61	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:534:NAG:C6	2:C:535:FUC:C1	2.78	0.61
1:B:382:ARG:HD2	3:B:178:HOH:O	2.00	0.61
2:E:2:GAL:O1	2:E:4:FUC:H5	2.00	0.61
1:I:234:VAL:HG13	3:I:536:HOH:O	2.00	0.61
1:A:469:GLN:HB2	1:A:520:TRP:CG	2.35	0.61
1:H:399:GLU:CB	1:H:400:PRO:HA	2.31	0.61
1:I:247:GLU:CB	3:I:538:HOH:O	2.49	0.61
1:I:337:THR:HG22	1:I:338:THR:OG1	2.00	0.60
1:A:390:GLN:HG2	1:A:444:TYR:C	2.22	0.60
1:H:268:THR:CG2	1:H:493:LYS:HA	2.31	0.60
1:H:494:SER:HB2	3:H:535:HOH:O	2.01	0.60
1:F:373:ASN:OD1	1:F:373:ASN:N	2.30	0.60
1:E:426:PHE:CD2	1:E:427:PRO:HD2	2.36	0.60
1:J:345:ARG:CG	1:J:345:ARG:NH2	2.46	0.60
1:E:280:PRO:HA	3:E:543:HOH:O	2.01	0.59
1:I:487:PHE:HA	3:I:537:HOH:O	2.03	0.59
2:F:2:GAL:O1	2:F:4:FUC:C5	2.46	0.59
1:F:390:GLN:CG	1:F:444:TYR:H	2.15	0.59
1:E:277:GLN:OE1	1:E:279:SER:HB3	2.03	0.59
1:E:341:ASP:HB3	1:E:343:SER:H	1.67	0.59
2:C:536:GAL:C1	2:C:537:BGC:H6	2.16	0.58
1:I:238:THR:HG22	1:I:239:ASN:O	2.03	0.58
1:B:353:THR:HG22	1:B:358:PHE:CE1	2.38	0.58
1:D:453:LEU:CD2	1:D:495:GLY:O	2.50	0.58
1:A:343:SER:HB3	1:C:444:TYR:CE1	2.38	0.58
1:A:472:VAL:HG13	1:A:490:LYS:HB3	1.85	0.58
1:F:328:GLY:HA3	1:F:400:PRO:HB3	1.85	0.58
1:A:390:GLN:HG3	1:A:444:TYR:H	1.68	0.58
1:F:260:GLN:HG3	1:F:421:ALA:HA	1.86	0.58
1:I:235:GLU:HG3	3:I:536:HOH:O	2.03	0.58
1:F:371:THR:O	1:F:371:THR:CG2	2.51	0.57
1:J:392:GLY:HA3	2:J:4:FUC:C1	2.34	0.57
1:E:277:GLN:HG3	1:E:306:GLN:HE22	1.67	0.57
1:G:443:GLY:N	2:G:1:FUC:H63	2.20	0.57
2:C:1:FUC:C5	2:C:2:GAL:O1	2.43	0.57
1:C:222:SER:HB2	3:C:538:HOH:O	2.04	0.57
1:J:356:VAL:HG23	1:J:411:ARG:HG3	1.87	0.57
1:G:319:ALA:HB1	1:G:320:PRO:HD2	1.86	0.57
1:H:288:GLY:HA3	1:H:302:ASN:O	2.04	0.57
1:B:277:GLN:OE1	1:B:279:SER:HB3	2.05	0.57
1:D:233:THR:HG21	1:D:512:ASN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:490:LYS:HG3	1:H:527:LEU:HD21	1.87	0.56
1:G:443:GLY:H	2:G:1:FUC:H63	1.69	0.56
1:C:390:GLN:HG3	1:C:444:TYR:H	1.70	0.56
1:E:463:GLN:HG2	3:E:541:HOH:O	2.05	0.56
1:C:360:PRO:HD2	1:C:408:TYR:O	2.05	0.56
2:F:2:GAL:C1	2:F:4:FUC:H5	2.35	0.56
1:G:453:LEU:CG	1:G:495:GLY:O	2.53	0.56
1:F:310:ASN:HB2	3:F:557:HOH:O	2.04	0.56
1:B:391:ASP:OD2	1:B:394:THR:HG23	2.05	0.56
2:C:3:NAG:C6	2:C:4:FUC:C1	2.72	0.56
1:H:493:LYS:HD2	3:H:533:HOH:O	2.05	0.56
1:G:523:GLN:HB2	3:G:546:HOH:O	2.05	0.56
1:A:232:LEU:HD21	1:C:463:GLN:NE2	2.20	0.56
1:E:229:VAL:HB	1:E:230:PRO:HD2	1.88	0.56
2:J:5:GAL:O6	2:J:6:BGC:H1	2.05	0.56
1:F:390:GLN:HG3	1:F:444:TYR:H	1.71	0.56
1:D:392:GLY:HA3	2:D:4:FUC:C1	2.35	0.56
3:D:111:HOH:O	1:F:279:SER:HB2	2.05	0.55
1:D:399:GLU:HB2	1:D:400:PRO:HA	1.89	0.55
2:D:5:GAL:C1	2:D:6:BGC:O6	2.54	0.55
1:B:287:ARG:NE	3:B:537:HOH:O	2.39	0.55
1:H:382:ARG:HB2	1:H:382:ARG:HH11	1.72	0.55
1:I:258:VAL:O	1:I:258:VAL:HG23	2.06	0.55
1:F:443:GLY:O	1:F:445:PRO:HD3	2.07	0.55
1:G:390:GLN:HG2	1:G:444:TYR:C	2.27	0.55
1:H:523:GLN:CB	3:H:537:HOH:O	2.54	0.55
1:H:399:GLU:N	3:H:91:HOH:O	2.40	0.54
1:F:371:THR:HG23	1:F:371:THR:O	2.06	0.54
1:H:231:ILE:CG2	3:H:545:HOH:O	2.54	0.54
1:H:376:GLU:CA	3:H:149:HOH:O	2.24	0.54
1:H:242:PHE:CD2	1:H:243:PRO:HD2	2.42	0.54
1:G:248:LYS:HE2	3:G:542:HOH:O	2.07	0.54
1:B:332:GLY:HA2	1:B:386:VAL:HG23	1.89	0.54
1:C:286:PHE:CD1	3:C:165:HOH:O	2.53	0.54
1:E:260:GLN:HG3	1:E:421:ALA:HA	1.90	0.54
1:E:260:GLN:HG3	1:E:421:ALA:CA	2.38	0.54
1:H:277:GLN:HG2	1:H:278:LEU:H	1.73	0.54
1:G:443:GLY:CA	2:G:1:FUC:C6	2.86	0.54
1:A:253:PRO:HD2	3:A:124:HOH:O	2.08	0.54
1:F:230:PRO:HG2	1:F:457:TRP:CD1	2.43	0.53
1:D:319:ALA:HB1	1:D:320:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HD12	1:B:319:ALA:O	2.08	0.53
1:B:417:HIS:HE1	3:B:49:HOH:O	1.91	0.53
2:D:1:FUC:H5	2:D:2:GAL:O1	2.09	0.53
2:J:2:GAL:O5	2:J:4:FUC:H5	2.08	0.53
1:A:392:GLY:HA3	2:C:535:FUC:O5	2.09	0.53
1:J:277:GLN:OE1	1:J:279:SER:N	2.41	0.53
1:C:523:GLN:NE2	3:C:557:HOH:O	2.42	0.53
1:G:232:LEU:HD21	1:J:463:GLN:NE2	2.24	0.53
1:E:433:PHE:HB3	1:E:450:ASP:HB3	1.90	0.53
1:G:244:ILE:HD12	1:G:436:SER:HB3	1.91	0.53
1:G:276:THR:HA	3:G:541:HOH:O	2.07	0.52
1:F:307:ASN:HD21	1:F:309:ASN:HB2	1.74	0.52
3:G:532:HOH:O	1:J:279:SER:HB2	2.09	0.52
1:C:523:GLN:HB3	3:C:183:HOH:O	2.09	0.52
1:A:226:PRO:HD2	3:A:533:HOH:O	2.10	0.52
1:I:430:GLN:NE2	1:I:503:GLY:H	2.06	0.52
1:J:285:THR:HG22	1:J:385:PRO:HD3	1.90	0.52
1:J:443:GLY:HA2	2:J:4:FUC:H63	1.91	0.52
1:I:377:THR:HG21	3:I:533:HOH:O	2.10	0.52
1:A:283:ILE:O	1:A:284:CYS:HB2	2.08	0.52
2:C:532:FUC:C6	2:C:535:FUC:H61	2.25	0.52
1:H:222:SER:H	1:H:469:GLN:HE22	1.58	0.52
1:D:283:ILE:O	1:D:284:CYS:HB2	2.10	0.52
1:H:530:MET:HA	3:H:546:HOH:O	2.10	0.52
1:I:485:VAL:HG12	3:I:544:HOH:O	2.09	0.51
1:H:376:GLU:CB	3:H:149:HOH:O	2.57	0.51
1:A:328:GLY:HA3	1:A:400:PRO:HB3	1.91	0.51
1:F:390:GLN:CG	1:F:444:TYR:N	2.74	0.51
2:E:6:BGC:H6C1	2:E:6:BGC:O1	2.09	0.51
1:B:277:GLN:HB2	1:B:321:LEU:HB3	1.93	0.51
1:G:472:VAL:CG1	1:G:490:LYS:HB3	2.40	0.51
1:I:238:THR:O	1:I:246:LEU:CD1	2.59	0.51
1:I:239:ASN:HA	1:I:246:LEU:HD21	1.92	0.51
1:E:390:GLN:HG3	1:E:444:TYR:N	2.24	0.51
1:D:272:LEU:O	1:D:273:LEU:HD23	2.11	0.51
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.75	0.51
1:H:231:ILE:CB	3:H:545:HOH:O	2.21	0.51
1:A:506:ASP:HB3	3:A:19:HOH:O	2.09	0.51
1:G:530:MET:HA	3:G:43:HOH:O	2.09	0.51
1:A:472:VAL:CG1	1:A:490:LYS:HB3	2.41	0.51
1:H:292:HIS:HB2	1:H:299:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:443:GLY:CA	2:G:1:FUC:H63	2.42	0.51
1:G:372:SER:C	1:G:373:ASN:HD22	2.15	0.50
2:D:2:GAL:C1	2:D:4:FUC:H5	2.41	0.50
1:H:340:ARG:HH11	1:H:340:ARG:CG	2.25	0.50
1:C:390:GLN:HG2	1:C:444:TYR:C	2.31	0.50
1:C:248:LYS:HE2	3:C:540:HOH:O	2.12	0.50
1:H:340:ARG:HG2	1:H:340:ARG:HH11	1.77	0.50
1:I:238:THR:C	1:I:246:LEU:CD1	2.80	0.50
1:B:358:PHE:C	1:B:360:PRO:HD3	2.31	0.50
1:I:529:PRO:O	1:I:530:MET:O	2.30	0.50
1:D:253:PRO:HD2	3:D:182:HOH:O	2.11	0.50
1:D:453:LEU:CG	1:D:495:GLY:O	2.60	0.50
2:E:6:BGC:H6C2	2:E:6:BGC:O1	2.10	0.50
1:H:221:GLU:N	1:H:469:GLN:HE21	2.08	0.50
1:H:382:ARG:CG	1:H:382:ARG:HH11	2.25	0.50
1:E:287:ARG:HD3	3:E:110:HOH:O	2.11	0.50
1:F:240:SER:OG	1:F:264:GLY:HA3	2.12	0.50
1:E:222:SER:HB3	3:E:93:HOH:O	2.11	0.50
1:F:230:PRO:HD3	1:F:460:HIS:CD2	2.47	0.50
1:I:384:THR:HG23	3:I:203:HOH:O	2.12	0.50
1:F:400:PRO:HD2	1:F:446:ASN:O	2.11	0.50
1:I:315:GLU:HB3	1:I:317:ILE:HG12	1.93	0.49
1:A:232:LEU:HD21	1:C:463:GLN:HE22	1.77	0.49
1:D:486:LEU:HD11	1:D:510:PRO:HD3	1.94	0.49
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.94	0.49
1:H:482:THR:OG1	1:H:484:ARG:HG2	2.12	0.49
1:B:481:ASP:OD2	1:B:512:ASN:ND2	2.44	0.49
1:F:399:GLU:HB2	1:F:400:PRO:HA	1.94	0.49
1:A:280:PRO:HG3	1:C:280:PRO:HG2	1.93	0.49
1:A:351:VAL:HB	1:A:367:PHE:CE1	2.47	0.49
1:E:268:THR:HG23	1:E:493:LYS:HA	1.92	0.49
1:G:344:THR:O	1:J:442:SER:HA	2.12	0.49
1:F:426:PHE:CE1	1:F:524:PHE:HA	2.47	0.49
1:J:360:PRO:HD2	1:J:408:TYR:O	2.13	0.49
1:G:373:ASN:N	1:G:373:ASN:HD22	2.09	0.49
1:E:390:GLN:HG2	1:E:444:TYR:C	2.32	0.49
1:J:392:GLY:HA3	2:J:4:FUC:O5	2.13	0.49
1:C:468:ALA:HA	1:C:520:TRP:CZ2	2.47	0.49
1:G:443:GLY:N	2:G:1:FUC:C6	2.74	0.49
1:F:443:GLY:C	1:F:445:PRO:HD3	2.33	0.49
1:A:327:VAL:HA	1:A:353:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:VAL:HG12	1:D:411:ARG:HG3	1.94	0.49
1:J:453:LEU:CD2	1:J:495:GLY:O	2.61	0.49
1:C:277:GLN:HG3	1:C:306:GLN:NE2	2.25	0.49
1:A:505:HIS:HE1	3:A:152:HOH:O	1.96	0.49
1:F:311:TYR:O	1:F:313:PRO:HD3	2.13	0.48
1:D:339:ARG:HG3	3:D:568:HOH:O	2.12	0.48
1:D:360:PRO:HD2	1:D:408:TYR:O	2.14	0.48
1:A:390:GLN:CD	1:A:391:ASP:O	2.51	0.48
1:E:438:MET:O	1:E:447:MET:HB3	2.13	0.48
1:G:334:LEU:O	1:G:346:GLY:HA2	2.14	0.48
1:F:390:GLN:HG3	1:F:444:TYR:N	2.29	0.48
1:I:424:PRO:C	1:I:426:PHE:H	2.17	0.48
1:A:391:ASP:CB	1:A:394:THR:HG23	2.41	0.48
1:G:345:ARG:HB3	2:J:1:FUC:H2	1.96	0.48
1:C:301:MET:HG2	1:C:303:LEU:HD23	1.95	0.48
1:H:476:ARG:HD3	1:H:518:ASP:OD2	2.13	0.48
1:D:523:GLN:HG2	3:D:532:HOH:O	2.13	0.48
1:D:472:VAL:HG11	1:D:490:LYS:HG2	1.95	0.47
1:F:490:LYS:O	1:F:497:VAL:HA	2.14	0.47
1:G:268:THR:HG23	1:G:493:LYS:HA	1.95	0.47
1:A:394:THR:O	1:A:395:THR:C	2.51	0.47
1:B:390:GLN:CG	1:B:444:TYR:H	2.27	0.47
1:E:277:GLN:HG3	1:E:306:GLN:NE2	2.30	0.47
1:D:328:GLY:HA3	1:D:400:PRO:HB3	1.96	0.47
1:H:511:PRO:HA	3:H:548:HOH:O	2.14	0.47
1:E:399:GLU:HB2	1:E:400:PRO:HA	1.96	0.47
1:E:390:GLN:CG	1:E:444:TYR:H	2.27	0.47
1:F:277:GLN:OE1	1:F:279:SER:HB3	2.13	0.47
1:I:288:GLY:HA3	1:I:302:ASN:O	2.14	0.47
1:G:399:GLU:HB2	1:G:400:PRO:HA	1.96	0.47
1:I:379:GLN:CB	3:I:205:HOH:O	2.62	0.47
2:G:1:FUC:H61	2:G:4:FUC:H61	1.96	0.47
2:J:2:GAL:O1	2:J:4:FUC:C5	2.56	0.47
1:C:425:THR:CA	3:C:551:HOH:O	2.55	0.47
1:A:359:THR:HB	1:A:362:LEU:HD12	1.96	0.47
1:G:426:PHE:CD2	1:G:427:PRO:HD2	2.49	0.47
1:C:489:CYS:HB2	1:C:498:THR:O	2.14	0.47
1:J:338:THR:HG21	1:J:345:ARG:NH1	2.27	0.47
1:F:414:HIS:ND1	2:G:5:GAL:H62	2.30	0.47
1:H:333:VAL:HG12	1:H:334:LEU:N	2.30	0.47
1:J:488:GLU:HG3	1:J:527:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:ARG:HG2	3:D:552:HOH:O	2.14	0.47
1:F:260:GLN:HG3	1:F:421:ALA:CA	2.44	0.47
1:G:372:SER:C	1:G:373:ASN:ND2	2.69	0.46
1:F:307:ASN:ND2	1:F:309:ASN:HB2	2.30	0.46
1:A:317:ILE:HD12	1:A:319:ALA:O	2.14	0.46
3:B:564:HOH:O	1:J:412:ASP:HA	2.15	0.46
1:J:390:GLN:HG2	1:J:445:PRO:N	2.30	0.46
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.49	0.46
1:A:490:LYS:HG3	1:A:527:LEU:HD11	1.95	0.46
1:H:382:ARG:CB	1:H:382:ARG:HH11	2.28	0.46
1:A:394:THR:HB	1:A:398:ASN:ND2	2.20	0.46
2:J:1:FUC:C5	2:J:4:FUC:H61	2.43	0.46
1:D:469:GLN:HG3	1:D:520:TRP:CD1	2.50	0.46
2:D:3:NAG:O6	2:D:4:FUC:C1	2.64	0.46
1:C:393:SER:HG	2:C:4:FUC:H2	1.79	0.46
1:D:390:GLN:HG2	1:D:445:PRO:HA	1.97	0.46
1:C:355:SER:HA	3:C:558:HOH:O	2.15	0.46
1:J:392:GLY:H	2:J:4:FUC:H2	1.81	0.46
1:H:382:ARG:CG	1:H:382:ARG:NH1	2.78	0.46
1:C:334:LEU:O	1:C:346:GLY:HA2	2.16	0.46
1:C:522:ASN:OD1	1:C:522:ASN:C	2.53	0.46
1:A:502:THR:HG23	3:A:559:HOH:O	2.16	0.45
1:B:394:THR:OG1	1:B:398:ASN:ND2	2.46	0.45
1:I:422:VAL:HG23	1:I:431:LEU:HD11	1.97	0.45
1:B:390:GLN:HG2	1:B:445:PRO:N	2.30	0.45
1:F:287:ARG:CD	3:F:532:HOH:O	2.62	0.45
1:G:261:PRO:O	1:G:265:ARG:NH1	2.49	0.45
1:I:330:ILE:HD12	1:I:353:THR:CG2	2.46	0.45
1:J:390:GLN:HE21	1:J:390:GLN:HB2	1.56	0.45
1:A:430:GLN:HG3	1:A:501:HIS:O	2.17	0.45
1:B:336:GLN:HG3	1:B:381:THR:OG1	2.16	0.45
1:D:277:GLN:OE1	1:D:279:SER:HB3	2.16	0.45
1:A:336:GLN:HE21	1:A:379:GLN:CB	2.17	0.45
1:H:468:ALA:HA	1:H:520:TRP:CZ2	2.52	0.45
1:J:248:LYS:HE2	3:J:542:HOH:O	2.17	0.45
1:B:332:GLY:HA3	1:B:384:THR:O	2.16	0.45
1:F:259:VAL:HG13	1:F:403:TRP:CZ3	2.52	0.45
1:G:327:VAL:HA	1:G:353:THR:OG1	2.17	0.45
1:C:344:THR:O	2:C:532:FUC:H2	2.16	0.45
1:A:390:GLN:HG3	1:A:444:TYR:N	2.32	0.45
1:C:523:GLN:CB	3:C:183:HOH:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:HIS:CD2	3:E:148:HOH:O	2.29	0.45
1:H:454:PRO:HG2	1:H:457:TRP:CD1	2.52	0.45
1:E:323:THR:HG22	1:E:324:PRO:O	2.16	0.45
1:G:343:SER:HB3	1:J:444:TYR:CE1	2.52	0.45
1:B:287:ARG:NH1	1:B:306:GLN:HA	2.32	0.45
1:H:359:THR:N	1:H:360:PRO:HD3	2.31	0.45
1:A:480:PRO:HG3	1:A:512:ASN:O	2.18	0.45
1:B:397:GLN:HB3	1:B:446:ASN:HB2	1.99	0.44
1:C:273:LEU:O	1:C:276:THR:HB	2.17	0.44
1:I:466:ALA:HA	1:I:467:PRO:HD3	1.87	0.44
1:E:435:ARG:HB2	1:E:450:ASP:OD1	2.16	0.44
1:D:390:GLN:HG3	1:D:444:TYR:H	1.82	0.44
1:E:319:ALA:HB1	1:E:320:PRO:HD2	1.99	0.44
2:C:532:FUC:C5	2:C:533:GAL:C2	2.90	0.44
1:G:279:SER:HB2	3:J:39:HOH:O	2.18	0.44
1:F:319:ALA:HB1	1:F:320:PRO:HD2	1.98	0.44
1:I:433:PHE:HB3	1:I:450:ASP:HB3	1.98	0.44
1:B:399:GLU:HB2	1:B:400:PRO:HA	1.98	0.44
1:F:478:VAL:HG21	1:F:516:ARG:NH1	2.32	0.44
1:F:516:ARG:HA	3:F:540:HOH:O	2.18	0.44
2:C:533:GAL:H62	2:C:535:FUC:H3	2.00	0.44
1:F:501:HIS:CD2	1:F:502:THR:N	2.86	0.44
1:B:442:SER:HA	1:E:344:THR:O	2.18	0.44
1:I:261:PRO:HG2	1:I:265:ARG:HD3	1.98	0.44
1:E:238:THR:N	1:E:456:GLU:OE1	2.47	0.44
1:C:276:THR:HA	3:C:550:HOH:O	2.18	0.44
1:E:476:ARG:HG3	1:E:485:VAL:HG11	2.00	0.44
1:J:328:GLY:HA3	1:J:400:PRO:HB3	2.00	0.44
1:G:225:LYS:HA	1:G:226:PRO:HD3	1.92	0.44
1:I:340:ARG:HG3	1:J:317:ILE:HG22	2.00	0.44
1:A:310:ASN:HA	3:A:549:HOH:O	2.18	0.44
1:D:346:GLY:N	1:F:441:CYS:O	2.51	0.44
1:H:277:GLN:HG3	1:H:306:GLN:NE2	2.33	0.43
1:F:307:ASN:O	1:F:308:TRP:HB2	2.17	0.43
1:D:486:LEU:CD1	1:D:510:PRO:HD3	2.48	0.43
1:B:308:TRP:CH2	1:B:380:ASN:HB3	2.53	0.43
1:E:230:PRO:HG2	1:E:457:TRP:CD1	2.53	0.43
1:G:430:GLN:HG3	1:G:501:HIS:O	2.18	0.43
1:B:287:ARG:CD	3:B:537:HOH:O	2.65	0.43
1:D:470:SER:OG	1:D:520:TRP:HB3	2.18	0.43
1:E:321:LEU:HD23	1:E:321:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:510:PRO:HA	1:F:511:PRO:HD3	1.81	0.43
1:G:472:VAL:HG11	1:G:490:LYS:HB3	1.99	0.43
2:G:1:FUC:H1	2:G:2:GAL:O3	2.19	0.43
1:I:260:GLN:HG3	1:I:421:ALA:HA	2.00	0.43
2:J:5:GAL:H2	2:J:6:BGC:C6	2.48	0.43
1:G:492:HIS:O	1:G:495:GLY:N	2.49	0.43
1:H:382:ARG:HG3	1:H:382:ARG:NH1	2.33	0.43
1:I:478:VAL:HG21	1:I:516:ARG:HD3	2.00	0.43
1:G:281:VAL:HG12	1:J:281:VAL:HG12	2.00	0.43
1:H:225:LYS:NZ	1:H:464:GLU:O	2.43	0.43
1:H:370:ASP:O	1:H:371:THR:C	2.56	0.43
1:H:369:THR:C	1:H:371:THR:H	2.22	0.43
1:C:425:THR:C	3:C:551:HOH:O	2.57	0.43
1:A:232:LEU:CD2	1:C:463:GLN:HE22	2.31	0.43
1:F:401:GLN:HA	3:F:199:HOH:O	2.19	0.43
1:D:390:GLN:O	1:D:443:GLY:HA3	2.19	0.43
1:E:377:THR:O	1:E:379:GLN:HG2	2.19	0.43
1:C:307:ASN:OD1	1:C:309:ASN:HB2	2.19	0.43
2:F:2:GAL:O6	2:F:2:GAL:O4	2.31	0.43
1:C:277:GLN:CG	1:C:306:GLN:HE22	2.28	0.42
1:G:344:THR:HG21	1:J:440:GLY:HA3	2.01	0.42
1:J:312:ASP:HA	1:J:313:PRO:HD3	1.90	0.42
1:I:419:ALA:HA	1:I:420:PRO:HD3	1.90	0.42
1:H:514:TYR:CD2	1:H:514:TYR:N	2.86	0.42
1:A:361:LYS:HG3	1:A:361:LYS:O	2.19	0.42
1:I:478:VAL:HG21	1:I:516:ARG:NH1	2.34	0.42
1:J:233:THR:HG21	1:J:512:ASN:HA	2.02	0.42
1:D:442:SER:OG	2:D:1:FUC:C1	2.66	0.42
1:G:336:GLN:OE1	1:G:345:ARG:HD2	2.20	0.42
1:E:471:ASP:HB2	3:E:553:HOH:O	2.17	0.42
1:F:512:ASN:N	1:F:512:ASN:OD1	2.51	0.42
2:E:5:GAL:O5	2:E:6:BGC:C3	2.65	0.42
1:I:306:GLN:C	1:I:308:TRP:H	2.21	0.42
1:C:431:LEU:HA	1:C:431:LEU:HD23	1.81	0.42
1:G:453:LEU:HG	1:G:495:GLY:O	2.19	0.42
1:C:523:GLN:CA	3:C:183:HOH:O	2.67	0.42
1:E:268:THR:CG2	1:E:493:LYS:HA	2.49	0.42
2:C:5:GAL:O1	2:C:6:BGC:O6	2.30	0.42
1:J:405:LEU:HD23	1:J:405:LEU:HA	1.69	0.42
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.54	0.42
1:I:258:VAL:O	1:I:258:VAL:CG2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:GLN:HG3	1:I:421:ALA:CA	2.50	0.42
1:E:469:GLN:HG3	1:E:520:TRP:CD1	2.55	0.42
1:G:360:PRO:HD2	1:G:408:TYR:O	2.20	0.42
1:H:530:MET:HG2	1:H:531:GLY:N	2.33	0.42
1:D:299:TYR:CE1	1:D:375:PHE:HB2	2.54	0.42
1:G:409:SER:CB	1:G:413:SER:HB2	2.43	0.42
1:I:241:ARG:NE	1:I:325:ASP:OD2	2.42	0.42
1:F:230:PRO:HD3	1:F:460:HIS:CG	2.54	0.41
1:B:283:ILE:O	1:B:284:CYS:HB2	2.20	0.41
1:G:328:GLY:HA3	1:G:400:PRO:HB3	2.01	0.41
1:G:240:SER:OG	1:G:264:GLY:HA3	2.20	0.41
1:F:287:ARG:NE	3:F:532:HOH:O	2.53	0.41
1:D:488:GLU:HG3	1:D:527:LEU:HD22	2.02	0.41
1:B:466:ALA:HA	1:B:467:PRO:HD2	1.92	0.41
2:D:5:GAL:H1	2:D:6:BGC:O6	2.20	0.41
1:A:454:PRO:HD2	1:A:457:TRP:CG	2.55	0.41
1:H:433:PHE:HB3	1:H:450:ASP:HB3	2.03	0.41
1:A:332:GLY:HA2	1:A:386:VAL:HG23	2.01	0.41
1:G:266:CYS:HA	1:G:271:ALA:O	2.21	0.41
1:B:430:GLN:HG3	1:B:501:HIS:O	2.20	0.41
1:F:391:ASP:HB3	1:F:394:THR:HG23	2.02	0.41
1:E:323:THR:HG23	1:E:324:PRO:HD2	2.01	0.41
1:G:253:PRO:HA	3:G:552:HOH:O	2.21	0.41
1:B:359:THR:N	1:B:360:PRO:HD3	2.36	0.41
1:G:232:LEU:HD21	1:J:463:GLN:HE21	1.86	0.41
1:G:307:ASN:OD1	1:G:309:ASN:HB2	2.21	0.41
1:D:285:THR:HG22	1:D:385:PRO:HD2	2.01	0.41
1:C:252:GLY:HA2	1:C:430:GLN:HE22	1.86	0.41
1:D:390:GLN:NE2	1:D:398:ASN:OD1	2.53	0.41
1:A:338:THR:OG1	1:A:345:ARG:NH2	2.47	0.41
1:G:469:GLN:CG	1:G:520:TRP:CD1	3.03	0.41
1:H:468:ALA:HA	1:H:520:TRP:CH2	2.55	0.41
1:G:414:HIS:O	1:G:415:ASN:C	2.57	0.41
1:J:433:PHE:HB3	1:J:450:ASP:HB3	2.03	0.41
1:B:461:PHE:O	1:B:462:TYR:C	2.59	0.41
1:F:327:VAL:HG23	1:F:404:VAL:O	2.20	0.41
1:C:246:LEU:HA	1:C:246:LEU:HD23	1.76	0.41
1:J:443:GLY:CA	2:J:4:FUC:H63	2.50	0.41
1:G:472:VAL:HG11	1:G:490:LYS:HD3	2.02	0.41
1:E:285:THR:HG22	1:E:385:PRO:CD	2.51	0.41
1:C:518:ASP:O	1:C:519:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:O	1:C:244:ILE:N	2.53	0.40
1:J:417:HIS:HE1	3:J:549:HOH:O	2.04	0.40
1:D:266:CYS:HB2	1:D:458:VAL:HG13	2.02	0.40
2:G:3:NAG:O7	2:G:3:NAG:O1	2.39	0.40
1:G:306:GLN:CB	3:G:89:HOH:O	2.68	0.40
1:D:453:LEU:HD11	1:D:495:GLY:O	2.21	0.40
1:F:319:ALA:HB1	1:F:320:PRO:CD	2.51	0.40
1:J:327:VAL:HG23	1:J:404:VAL:O	2.21	0.40
1:D:522:ASN:HB2	3:D:77:HOH:O	2.21	0.40
1:C:279:SER:HA	1:C:280:PRO:HD3	1.93	0.40
1:D:319:ALA:HB1	1:D:320:PRO:CD	2.50	0.40
1:G:396:HIS:O	1:G:397:GLN:HB2	2.22	0.40
1:G:443:GLY:CA	2:G:1:FUC:H61	2.48	0.40
1:A:426:PHE:CE1	1:A:524:PHE:HA	2.56	0.40
1:E:505:HIS:HE1	3:E:12:HOH:O	2.04	0.40
1:E:327:VAL:HA	1:E:353:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
1	F	306/311 (98%)	290 (95%)	16 (5%)	0	100	100
1	G	306/311 (98%)	295 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	294/311 (94%)	278 (95%)	16 (5%)	0	100	100
1	I	274/311 (88%)	252 (92%)	20 (7%)	2 (1%)	26	67
1	J	305/311 (98%)	295 (97%)	10 (3%)	0	100	100
All	All	3018/3110 (97%)	2878 (95%)	138 (5%)	2 (0%)	56	89

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%)	24	61
1	B	268/272 (98%)	247 (92%)	21 (8%)	16	48
1	C	271/272 (100%)	248 (92%)	23 (8%)	13	43
1	D	268/272 (98%)	250 (93%)	18 (7%)	20	55
1	E	271/272 (100%)	248 (92%)	23 (8%)	13	43
1	F	269/272 (99%)	252 (94%)	17 (6%)	22	58
1	G	266/272 (98%)	245 (92%)	21 (8%)	15	47
1	H	249/272 (92%)	228 (92%)	21 (8%)	14	43
1	I	219/272 (80%)	199 (91%)	20 (9%)	12	39
1	J	267/272 (98%)	244 (91%)	23 (9%)	13	42
All	All	2617/2720 (96%)	2414 (92%)	203 (8%)	16	48

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LYS

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Mol	Chain	Res	Type
1	A	277	GLN
1	A	282	ASP
1	A	287	ARG
1	A	340	ARG
1	A	364	SER
1	A	372	SER
1	A	373	ASN
1	A	390	GLN
1	A	470	SER
1	A	476	ARG
1	A	486	LEU
1	A	494	SER
1	A	499	VAL
1	A	516	ARG
1	A	522	ASN
1	B	248	LYS
1	B	255	SER
1	B	277	GLN
1	B	282	ASP
1	B	287	ARG
1	B	290	VAL
1	B	305	SER
1	B	331	GLN
1	B	364	SER
1	B	382	ARG
1	B	390	GLN
1	B	393	SER
1	B	395	THR
1	B	413	SER
1	B	472	VAL
1	B	476	ARG
1	B	482	THR
1	B	486	LEU
1	B	494	SER
1	B	522	ASN
1	B	530	MET
1	C	224	THR
1	C	248	LYS
1	C	277	GLN
1	C	287	ARG
1	C	297	GLN
1	C	305	SER

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Mol	Chain	Res	Type
1	C	310	ASN
1	C	340	ARG
1	C	345	ARG
1	C	355	SER
1	C	364	SER
1	C	372	SER
1	C	382	ARG
1	C	390	GLN
1	C	393	SER
1	C	413	SER
1	C	416	VAL
1	C	442	SER
1	C	465	SER
1	C	484	ARG
1	C	486	LEU
1	C	493	LYS
1	C	530	MET
1	D	248	LYS
1	D	277	GLN
1	D	282	ASP
1	D	287	ARG
1	D	345	ARG
1	D	364	SER
1	D	372	SER
1	D	373	ASN
1	D	374	ASP
1	D	382	ARG
1	D	390	GLN
1	D	412	ASP
1	D	476	ARG
1	D	484	ARG
1	D	486	LEU
1	D	494	SER
1	D	499	VAL
1	D	530	MET
1	E	224	THR
1	E	248	LYS
1	E	277	GLN
1	E	287	ARG
1	E	305	SER
1	E	331	GLN
1	E	339	ARG

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Mol	Chain	Res	Type
1	E	340	ARG
1	E	341	ASP
1	E	343	SER
1	E	362	LEU
1	E	364	SER
1	E	372	SER
1	E	374	ASP
1	E	382	ARG
1	E	390	GLN
1	E	393	SER
1	E	397	GLN
1	E	412	ASP
1	E	413	SER
1	E	416	VAL
1	E	486	LEU
1	E	493	LYS
1	F	248	LYS
1	F	277	GLN
1	F	287	ARG
1	F	305	SER
1	F	331	GLN
1	F	345	ARG
1	F	364	SER
1	F	371	THR
1	F	372	SER
1	F	390	GLN
1	F	393	SER
1	F	412	ASP
1	F	416	VAL
1	F	442	SER
1	F	484	ARG
1	F	486	LEU
1	F	530	MET
1	G	224	THR
1	G	277	GLN
1	G	282	ASP
1	G	287	ARG
1	G	290	VAL
1	G	309	ASN
1	G	331	GLN
1	G	364	SER
1	G	372	SER

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Mol	Chain	Res	Type
1	G	373	ASN
1	G	374	ASP
1	G	376	GLU
1	G	381	THR
1	G	390	GLN
1	G	393	SER
1	G	395	THR
1	G	413	SER
1	G	435	ARG
1	G	442	SER
1	G	484	ARG
1	G	486	LEU
1	H	248	LYS
1	H	277	GLN
1	H	310	ASN
1	H	329	LYS
1	H	331	GLN
1	H	337	THR
1	H	340	ARG
1	H	355	SER
1	H	364	SER
1	H	375	PHE
1	H	377	THR
1	H	382	ARG
1	H	384	THR
1	H	399	GLU
1	H	413	SER
1	H	441	CYS
1	H	471	ASP
1	H	484	ARG
1	H	486	LEU
1	H	494	SER
1	H	504	GLN
1	I	223	ARG
1	I	225	LYS
1	I	234	VAL
1	I	257	PHE
1	I	277	GLN
1	I	289	ASP
1	I	312	ASP
1	I	331	GLN
1	I	337	THR

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Mol	Chain	Res	Type
1	I	377	THR
1	I	384	THR
1	I	388	VAL
1	I	413	SER
1	I	437	THR
1	I	471	ASP
1	I	484	ARG
1	I	486	LEU
1	I	494	SER
1	I	526	THR
1	I	530	MET
1	J	225	LYS
1	J	277	GLN
1	J	282	ASP
1	J	287	ARG
1	J	290	VAL
1	J	305	SER
1	J	309	ASN
1	J	338	THR
1	J	339	ARG
1	J	340	ARG
1	J	343	SER
1	J	345	ARG
1	J	364	SER
1	J	376	GLU
1	J	382	ARG
1	J	390	GLN
1	J	393	SER
1	J	413	SER
1	J	416	VAL
1	J	481	ASP
1	J	484	ARG
1	J	486	LEU
1	J	494	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	A	390	GLN
1	A	396	HIS
1	A	398	ASN

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Mol	Chain	Res	Type
1	A	505	HIS
1	B	390	GLN
1	B	417	HIS
1	C	306	GLN
1	C	463	GLN
1	C	505	HIS
1	C	523	GLN
1	D	306	GLN
1	D	310	ASN
1	D	446	ASN
1	E	306	GLN
1	E	414	HIS
1	E	417	HIS
1	E	505	HIS
1	F	297	GLN
1	F	347	HIS
1	F	390	GLN
1	F	501	HIS
1	F	505	HIS
1	G	373	ASN
1	H	306	GLN
1	H	347	HIS
1	H	469	GLN
1	I	430	GLN
1	I	469	GLN
1	J	390	GLN
1	J	398	ASN
1	J	417	HIS

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	0.54	0	16,16,16	0.84	1 (6%)
2	GAL	B	2	2	11,11,12	0.70	1 (9%)	15,15,17	0.96	1 (6%)
2	NAG	B	3	2	14,14,15	0.61	0	12,19,21	1.24	2 (16%)
2	FUC	B	4	2	10,10,11	0.43	0	14,14,16	1.01	1 (7%)
2	GAL	B	5	2	11,11,12	0.58	0	12,15,17	1.13	2 (16%)
2	BGC	B	6	2	11,11,12	0.56	0	15,15,17	0.99	2 (13%)
2	FUC	C	1	2	11,11,11	1.74	3 (27%)	16,16,16	3.50	6 (37%)
2	GAL	C	2	2	11,11,12	1.95	4 (36%)	15,15,17	2.25	5 (33%)
2	NAG	C	3	2	14,14,15	1.02	1 (7%)	12,19,21	3.60	3 (25%)
2	FUC	C	4	2	10,10,11	1.46	2 (20%)	14,14,16	2.92	7 (50%)
2	GAL	C	5	2	11,11,12	0.56	0	12,15,17	2.18	2 (16%)
2	FUC	C	532	2	11,11,11	1.20	1 (9%)	16,16,16	3.20	5 (31%)
2	GAL	C	533	2	11,11,12	1.42	2 (18%)	15,15,17	2.57	7 (46%)
2	NAG	C	534	2	14,14,15	0.96	0	12,19,21	4.54	3 (25%)
2	FUC	C	535	2	10,10,11	0.42	0	14,14,16	1.03	1 (7%)
2	GAL	C	536	2	11,11,12	0.56	0	12,15,17	1.16	2 (16%)
2	BGC	C	537	2	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
2	BGC	C	6	2	11,11,12	0.53	0	15,15,17	2.01	5 (33%)
2	FUC	D	1	2	11,11,11	0.56	0	16,16,16	0.79	1 (6%)
2	GAL	D	2	2	11,11,12	1.95	6 (54%)	15,15,17	3.51	6 (40%)
2	NAG	D	3	2	14,14,15	1.27	1 (7%)	12,19,21	5.16	4 (33%)
2	FUC	D	4	2	10,10,11	0.48	0	14,14,16	1.13	2 (14%)
2	GAL	D	5	2	11,11,12	0.83	0	12,15,17	2.94	3 (25%)
2	BGC	D	6	2	11,11,12	1.19	2 (18%)	15,15,17	2.55	6 (40%)
2	FUC	E	1	2	11,11,11	0.73	0	16,16,16	0.96	1 (6%)
2	GAL	E	2	2	11,11,12	1.94	4 (36%)	15,15,17	2.19	6 (40%)
2	NAG	E	3	2	14,14,15	0.94	0	12,19,21	2.81	2 (16%)
2	FUC	E	4	2	10,10,11	0.42	0	14,14,16	1.01	1 (7%)
2	GAL	E	5	2	11,11,12	1.21	2 (18%)	12,15,17	2.54	5 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	E	6	2	11,11,12	1.22	1 (9%)	15,15,17	2.54	6 (40%)
2	FUC	F	1	2	11,11,11	0.54	0	16,16,16	0.84	1 (6%)
2	GAL	F	2	2	11,11,12	0.69	0	15,15,17	0.96	1 (6%)
2	NAG	F	3	2	14,14,15	0.59	0	12,19,21	1.23	2 (16%)
2	FUC	F	4	2	10,10,11	0.44	0	14,14,16	1.01	1 (7%)
2	GAL	F	5	2	11,11,12	0.58	0	12,15,17	1.14	2 (16%)
2	BGC	F	6	2	11,11,12	0.57	0	15,15,17	1.01	2 (13%)
2	FUC	G	1	2	11,11,11	0.53	0	16,16,16	0.84	1 (6%)
2	GAL	G	2	2	11,11,12	0.70	1 (9%)	15,15,17	0.95	1 (6%)
2	NAG	G	3	2	14,14,15	0.60	0	12,19,21	1.24	2 (16%)
2	FUC	G	4	2	10,10,11	0.43	0	14,14,16	1.01	1 (7%)
2	GAL	G	5	2	11,11,12	0.58	0	12,15,17	1.16	2 (16%)
2	BGC	G	6	2	11,11,12	0.57	0	15,15,17	0.99	2 (13%)
2	FUC	J	1	2	11,11,11	0.54	0	16,16,16	0.84	1 (6%)
2	GAL	J	2	2	11,11,12	0.70	1 (9%)	15,15,17	0.96	1 (6%)
2	NAG	J	3	2	14,14,15	0.60	0	12,19,21	1.23	2 (16%)
2	FUC	J	4	2	10,10,11	0.43	0	14,14,16	1.01	1 (7%)
2	GAL	J	5	2	11,11,12	0.58	0	12,15,17	1.14	2 (16%)
2	BGC	J	6	2	11,11,12	0.56	0	15,15,17	0.99	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	FUC	O5-C5	-3.68	1.35	1.44
2	D	3	NAG	C3-C4	-3.68	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	GAL	O5-C1	-3.65	1.36	1.43
2	E	2	GAL	O5-C5	-3.63	1.35	1.44
2	C	2	GAL	O5-C5	-3.35	1.36	1.44
2	D	2	GAL	C3-C4	-3.24	1.48	1.52
2	C	533	GAL	O5-C1	-3.17	1.37	1.43
2	C	532	FUC	O5-C1	-3.16	1.37	1.43
2	C	2	GAL	O5-C1	-3.09	1.37	1.43
2	C	2	GAL	C2-C3	-2.83	1.48	1.52
2	D	2	GAL	O5-C1	-2.78	1.37	1.43
2	C	1	FUC	C4-C5	-2.70	1.47	1.52
2	C	4	FUC	O5-C1	-2.63	1.39	1.43
2	C	3	NAG	C4-C5	-2.59	1.47	1.52
2	C	533	GAL	O5-C5	-2.53	1.38	1.44
2	D	2	GAL	O5-C5	-2.43	1.38	1.44
2	E	5	GAL	C1-C2	-2.40	1.51	1.52
2	D	2	GAL	C4-C5	-2.26	1.48	1.53
2	D	6	BGC	O5-C5	-2.25	1.40	1.44
2	D	6	BGC	C1-C2	-2.23	1.48	1.52
2	D	2	GAL	O3-C3	-2.15	1.38	1.43
2	E	5	GAL	O5-C1	-2.15	1.39	1.43
2	C	1	FUC	O4-C4	-2.14	1.37	1.43
2	E	2	GAL	C3-C4	-2.03	1.49	1.52
2	C	4	FUC	C1-C2	-2.01	1.47	1.52
2	G	2	GAL	O1-C1	2.02	1.44	1.39
2	B	2	GAL	O1-C1	2.02	1.44	1.39
2	E	2	GAL	O1-C1	2.02	1.44	1.39
2	D	2	GAL	O1-C1	2.02	1.44	1.39
2	J	2	GAL	O1-C1	2.03	1.44	1.39
2	C	2	GAL	O1-C1	2.03	1.44	1.39
2	E	6	BGC	C4-C5	2.93	1.60	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	NAG	C6-C5-C4	-16.97	91.65	113.29
2	C	534	NAG	C6-C5-C4	-14.77	94.45	113.29
2	C	3	NAG	C6-C5-C4	-10.98	99.29	113.29
2	D	2	GAL	O5-C1-C2	-9.99	102.95	110.72
2	C	532	FUC	O5-C1-C2	-9.61	94.48	109.80
2	C	1	FUC	C6-C5-C4	-9.22	94.92	113.08
2	D	5	GAL	C6-C5-C4	-9.00	101.81	113.29
2	E	3	NAG	C6-C5-C4	-8.79	102.08	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	FUC	O5-C5-C4	-7.31	96.85	109.53
2	C	4	FUC	C6-C5-C4	-6.19	100.90	113.08
2	E	6	BGC	O5-C5-C6	-6.17	99.05	106.62
2	C	5	GAL	C6-C5-C4	-6.17	105.42	113.29
2	C	4	FUC	O5-C1-C2	-6.10	100.97	110.86
2	C	1	FUC	O5-C1-C2	-5.93	100.34	109.80
2	E	5	GAL	C6-C5-C4	-5.86	105.82	113.29
2	D	6	BGC	C4-C5-C6	-5.83	101.63	112.38
2	D	2	GAL	C1-O5-C5	-5.69	102.93	113.42
2	C	533	GAL	C1-O5-C5	-5.30	103.65	113.42
2	C	2	GAL	C1-O5-C5	-5.30	103.66	113.42
2	D	2	GAL	C6-C5-C4	-5.14	100.33	113.02
2	C	532	FUC	O5-C5-C4	-5.03	100.81	109.53
2	D	6	BGC	C1-O5-C5	-4.81	104.60	113.47
2	C	533	GAL	C6-C5-C4	-4.41	102.14	113.02
2	C	534	NAG	C3-C2-N2	-4.35	102.99	110.59
2	C	3	NAG	C2-N2-C7	-4.18	117.67	123.04
2	E	5	GAL	C1-O5-C5	-4.18	105.75	113.47
2	C	2	GAL	O5-C5-C4	-4.04	102.10	109.68
2	E	2	GAL	O3-C3-C4	-4.04	101.99	110.12
2	E	2	GAL	C1-O5-C5	-3.75	106.50	113.42
2	D	3	NAG	C3-C2-N2	-3.63	104.25	110.59
2	E	2	GAL	O5-C5-C4	-3.52	103.07	109.68
2	D	6	BGC	O1-C1-C2	-3.38	100.15	109.21
2	C	3	NAG	C3-C2-N2	-3.33	104.77	110.59
2	C	5	GAL	O5-C1-C2	-3.23	104.74	109.81
2	C	533	GAL	O1-C1-O5	-3.18	101.08	108.28
2	C	4	FUC	O3-C3-C4	-3.13	103.29	110.34
2	C	532	FUC	O2-C2-C3	-3.11	103.34	110.34
2	C	536	GAL	C6-C5-C4	-3.06	109.39	113.29
2	G	5	GAL	C6-C5-C4	-3.03	109.43	113.29
2	D	6	BGC	C3-C4-C5	-3.00	105.32	111.40
2	B	3	NAG	C6-C5-C4	-2.98	109.49	113.29
2	F	3	NAG	C6-C5-C4	-2.97	109.50	113.29
2	F	5	GAL	C6-C5-C4	-2.97	109.51	113.29
2	J	3	NAG	C6-C5-C4	-2.96	109.51	113.29
2	J	5	GAL	C6-C5-C4	-2.95	109.53	113.29
2	G	3	NAG	C6-C5-C4	-2.94	109.53	113.29
2	D	2	GAL	O3-C3-C4	-2.94	104.21	110.12
2	B	5	GAL	C6-C5-C4	-2.93	109.55	113.29
2	C	4	FUC	O2-C2-C1	-2.92	103.36	109.21
2	D	6	BGC	O2-C2-C1	-2.91	103.42	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	BGC	C1-O5-C5	-2.88	108.17	113.47
2	E	5	GAL	O5-C1-C2	-2.83	105.37	109.81
2	D	5	GAL	C1-O5-C5	-2.80	108.29	113.47
2	E	2	GAL	O4-C4-C3	-2.78	104.97	110.00
2	D	6	BGC	O5-C5-C4	-2.77	104.80	109.97
2	C	6	BGC	O5-C5-C4	-2.74	104.87	109.97
2	C	532	FUC	O1-C1-C2	-2.72	101.92	109.21
2	C	2	GAL	O3-C3-C2	-2.70	103.44	110.06
2	D	2	GAL	O5-C5-C4	-2.58	104.85	109.68
2	D	5	GAL	O5-C1-C2	-2.57	105.78	109.81
2	E	6	BGC	O3-C3-C4	-2.54	103.84	110.06
2	C	1	FUC	O4-C4-C5	-2.51	103.94	109.84
2	C	533	GAL	O3-C3-C2	-2.51	103.91	110.06
2	C	537	BGC	C1-O5-C5	-2.44	108.97	113.47
2	C	2	GAL	O4-C4-C3	-2.42	105.63	110.00
2	C	533	GAL	O5-C1-C2	-2.39	108.86	110.72
2	C	6	BGC	C1-O5-C5	-2.25	109.31	113.47
2	C	4	FUC	C1-O5-C5	-2.25	108.91	112.38
2	G	1	FUC	C1-O5-C5	-2.19	109.47	113.57
2	B	1	FUC	C1-O5-C5	-2.19	109.47	113.57
2	F	1	FUC	C1-O5-C5	-2.19	109.48	113.57
2	B	3	NAG	C1-O5-C5	-2.18	109.44	113.47
2	C	1	FUC	O1-C1-C2	-2.18	103.38	109.21
2	J	1	FUC	C1-O5-C5	-2.17	109.50	113.57
2	G	5	GAL	C1-O5-C5	-2.17	109.45	113.47
2	J	5	GAL	C1-O5-C5	-2.17	109.45	113.47
2	G	3	NAG	C1-O5-C5	-2.16	109.47	113.47
2	F	3	NAG	C1-O5-C5	-2.15	109.49	113.47
2	G	6	BGC	C1-O5-C5	-2.15	109.50	113.47
2	F	5	GAL	C1-O5-C5	-2.15	109.49	113.47
2	D	1	FUC	C1-O5-C5	-2.15	109.54	113.57
2	J	6	BGC	C1-O5-C5	-2.15	109.51	113.47
2	B	6	BGC	C1-O5-C5	-2.15	109.51	113.47
2	C	4	FUC	O4-C4-C3	-2.15	105.51	110.34
2	D	3	NAG	C1-O5-C5	-2.14	109.52	113.47
2	J	3	NAG	C1-O5-C5	-2.14	109.52	113.47
2	E	2	GAL	C6-C5-C4	-2.13	107.75	113.02
2	B	2	GAL	C1-O5-C5	-2.13	109.49	113.42
2	B	5	GAL	C1-O5-C5	-2.13	109.54	113.47
2	F	2	GAL	C1-O5-C5	-2.12	109.51	113.42
2	C	534	NAG	O5-C5-C6	-2.12	100.99	106.36
2	G	2	GAL	C1-O5-C5	-2.12	109.52	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	GAL	C1-O5-C5	-2.12	109.52	113.42
2	E	5	GAL	O2-C2-C3	-2.10	104.92	110.06
2	F	6	BGC	C1-O5-C5	-2.09	109.62	113.47
2	C	6	BGC	O1-C1-O5	-2.06	104.60	110.25
2	C	535	FUC	C1-O5-C5	-2.04	109.23	112.38
2	C	536	GAL	C1-O5-C5	-2.04	109.70	113.47
2	C	1	FUC	O2-C2-C3	-2.03	105.76	110.34
2	D	2	GAL	O4-C4-C3	-2.00	106.39	110.00
2	F	4	FUC	O5-C5-C6	2.01	109.45	106.13
2	J	4	FUC	O5-C5-C6	2.01	109.46	106.13
2	C	537	BGC	O5-C5-C6	2.02	109.09	106.62
2	B	4	FUC	O5-C5-C6	2.04	109.50	106.13
2	G	4	FUC	O5-C5-C6	2.05	109.52	106.13
2	D	4	FUC	O5-C5-C6	2.05	109.52	106.13
2	E	4	FUC	O5-C5-C6	2.05	109.53	106.13
2	C	2	GAL	O5-C1-C2	2.12	112.38	110.72
2	E	1	FUC	O5-C5-C6	2.24	111.52	106.64
2	D	3	NAG	O5-C5-C6	2.27	112.09	106.36
2	D	4	FUC	C1-C2-C3	2.31	112.28	109.54
2	B	6	BGC	O5-C5-C6	2.35	109.50	106.62
2	G	6	BGC	O5-C5-C6	2.36	109.51	106.62
2	J	6	BGC	O5-C5-C6	2.38	109.53	106.62
2	F	6	BGC	O5-C5-C6	2.42	109.59	106.62
2	E	5	GAL	O5-C5-C6	2.46	112.57	106.36
2	C	4	FUC	O5-C5-C6	2.56	110.37	106.13
2	E	6	BGC	C4-C3-C2	2.62	114.12	110.56
2	E	3	NAG	O4-C4-C5	2.79	115.50	109.88
2	C	533	GAL	O5-C5-C4	2.82	114.97	109.68
2	C	6	BGC	O5-C1-C2	2.98	114.55	109.80
2	E	2	GAL	C3-C4-C5	3.02	112.98	109.93
2	C	533	GAL	C3-C4-C5	3.11	113.06	109.93
2	E	6	BGC	C3-C4-C5	3.22	117.94	111.40
2	C	532	FUC	C4-C3-C2	3.82	117.92	110.79
2	C	6	BGC	O5-C5-C6	3.98	111.49	106.62
2	E	6	BGC	O5-C5-C4	4.22	117.82	109.97

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
2	J	4	FUC	13	0
2	J	5	GAL	6	0
2	J	6	BGC	6	0

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.76	0 100 100	10, 22, 54, 90	0
1	B	307/311 (98%)	-0.68	0 100 100	15, 26, 51, 65	0
1	C	311/311 (100%)	-0.53	0 100 100	13, 27, 49, 64	0
1	D	307/311 (98%)	-0.57	1 (0%) 94 84	11, 27, 59, 82	0
1	E	309/311 (99%)	-0.57	2 (0%) 90 74	15, 28, 60, 74	0
1	F	308/311 (99%)	-0.45	0 100 100	20, 39, 68, 83	0
1	G	308/311 (99%)	-0.41	1 (0%) 94 84	22, 38, 63, 104	0
1	H	300/311 (96%)	-0.25	0 100 100	17, 41, 79, 109	0
1	I	284/311 (91%)	0.88	35 (12%) 5 2	51, 81, 110, 140	0
1	J	307/311 (98%)	-0.57	0 100 100	17, 33, 62, 79	0
All	All	3050/3110 (98%)	-0.40	39 (1%) 79 53	10, 33, 83, 140	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	300	THR	4.0
1	I	296	THR	4.0
1	I	411	ARG	3.3
1	I	293	ILE	3.2
1	G	413	SER	3.2
1	I	474	LEU	3.1
1	I	481	ASP	3.1
1	I	427	PRO	3.1
1	I	377	THR	3.0
1	I	369	THR	2.8
1	I	289	ASP	2.8
1	I	524	PHE	2.8
1	I	292	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	297	GLN	2.7
1	I	346	GLY	2.7
1	I	362	LEU	2.7
1	I	310	ASN	2.6
1	I	376	GLU	2.5
1	I	261	PRO	2.5
1	I	298	ASN	2.4
1	I	294	ALA	2.4
1	I	290	VAL	2.3
1	I	425	THR	2.3
1	I	375	PHE	2.3
1	I	295	GLY	2.3
1	I	364	SER	2.3
1	I	506	ASP	2.3
1	I	299	TYR	2.2
1	I	412	ASP	2.2
1	I	314	THR	2.2
1	D	393	SER	2.2
1	I	366	GLN	2.2
1	I	526	THR	2.2
1	I	359	THR	2.1
1	I	382	ARG	2.1
1	I	347	HIS	2.1
1	E	482	THR	2.1
1	E	484	ARG	2.0
1	I	330	ILE	2.0

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. 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(\AA^2)	Q<0.9
2	FUC	F	4	10/11	0.70	0.54	18.49	119,120,121,121	0
2	BGC	E	6	11/12	0.73	0.64	11.91	108,109,109,109	0
2	FUC	J	4	10/11	0.75	0.53	7.89	107,108,109,109	0
2	FUC	B	4	10/11	0.76	0.38	7.24	99,100,101,101	0
2	FUC	G	4	10/11	0.78	0.42	5.78	100,101,102,102	0
2	FUC	C	4	10/11	0.77	0.33	5.19	92,96,97,98	0
2	FUC	B	1	11/11	0.81	0.30	3.60	74,77,80,84	0
2	FUC	C	535	10/11	0.70	0.44	3.22	91,93,94,95	0
2	FUC	E	4	10/11	0.86	0.34	2.98	73,75,76,77	0
2	FUC	D	1	11/11	0.81	0.33	2.93	84,87,89,92	0
2	FUC	G	1	11/11	0.79	0.26	2.59	70,74,79,85	0
2	FUC	J	1	11/11	0.84	0.31	2.42	83,84,88,92	0
2	FUC	E	1	11/11	0.87	0.23	2.36	57,61,63,68	0
2	FUC	D	4	10/11	0.77	0.40	1.76	97,99,99,99	0
2	FUC	F	1	11/11	0.86	0.31	1.71	100,101,104,108	0
2	FUC	C	532	11/11	0.86	0.31	1.40	73,74,79,83	0
2	FUC	C	1	11/11	0.86	0.20	1.17	71,72,78,85	0
2	GAL	B	5	11/12	0.65	0.51	-	118,119,123,126	0
2	GAL	C	533	11/12	0.76	0.39	-	85,88,90,93	0
2	GAL	J	5	11/12	0.71	0.48	-	122,123,126,129	0
2	GAL	D	2	11/12	0.79	0.40	-	92,94,96,100	0
2	NAG	E	3	14/15	0.83	0.45	-	81,83,88,93	0
2	NAG	B	3	14/15	0.82	0.47	-	101,104,108,113	0
2	BGC	B	6	11/12	0.54	0.64	-	129,130,130,131	0
2	NAG	D	3	14/15	0.84	0.43	-	97,102,106,111	0
2	GAL	F	2	11/12	0.77	0.42	-	111,112,114,117	0
2	BGC	F	6	11/12	0.69	0.44	-	134,136,136,136	0
2	NAG	F	3	14/15	0.82	0.40	-	120,121,124,126	0
2	GAL	E	2	11/12	0.87	0.33	-	71,73,75,79	0
2	GAL	E	5	11/12	0.76	0.63	-	96,98,101,105	0
2	NAG	J	3	14/15	0.82	0.47	-	109,111,114,119	0
2	GAL	C	5	11/12	0.54	0.52	-	115,117,120,124	0
2	GAL	B	2	11/12	0.87	0.38	-	88,91,92,98	0
2	NAG	G	3	14/15	0.67	0.36	-	97,103,106,110	0
2	BGC	G	6	11/12	0.61	0.62	-	113,116,117,117	0
2	BGC	C	6	11/12	0.50	0.77	-	128,130,130,130	0
2	BGC	C	537	11/12	0.69	0.61	-	123,125,126,126	0
2	GAL	C	2	11/12	0.87	0.32	-	89,92,93,98	0
2	NAG	C	3	14/15	0.81	0.41	-	99,103,106,111	0
2	NAG	C	534	14/15	0.82	0.40	-	94,97,103,108	0
2	GAL	G	2	11/12	0.84	0.30	-	93,96,97,99	0
2	GAL	G	5	11/12	0.69	0.44	-	112,113,114,116	0
2	GAL	D	5	11/12	0.67	0.51	-	114,116,120,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BGC	D	6	11/12	0.78	0.60	-	124,126,126,127	0
2	GAL	C	536	11/12	0.53	0.61	-	113,115,118,122	0
2	BGC	J	6	11/12	0.65	0.69	-	132,133,133,133	0
2	GAL	J	2	11/12	0.84	0.35	-	95,96,99,104	0
2	GAL	F	5	11/12	0.65	0.36	-	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.