Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:18 PM GMT

PDB ID	:	3SLN
Title	:	Structural characterization of a GII.4 2004 norovirus variant (TCH05) bound to H pentasaccharide
Authors	:	Shanker, S.; Choi, J-M.; Sankaran, B.; Atmar, R.L.; Estes M.K.; Prasad B.V.V.
Deposited on	:	2011-06-24
Resolution	:	2.84 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

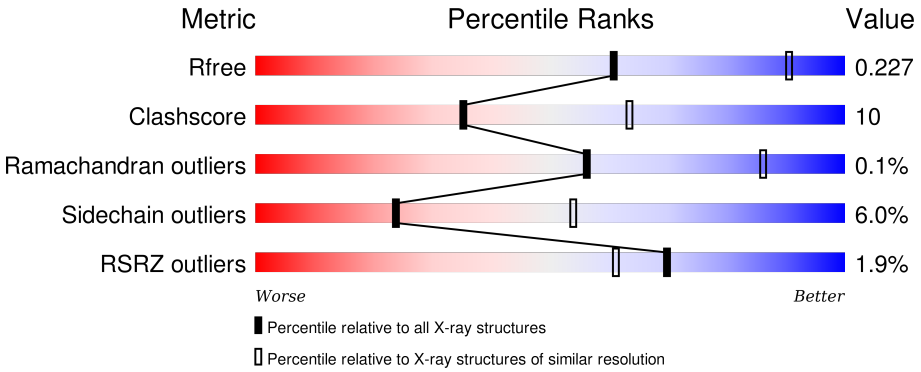
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.84 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}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 <=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	84% 14%
1	B	311	80% 16%
1	C	311	82% 16%
1	D	311	83% 13%
1	E	311	80% 18%

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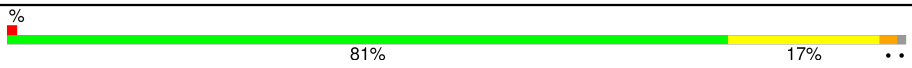
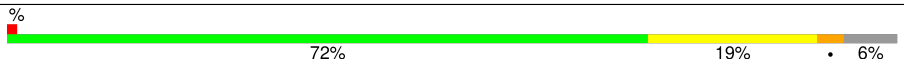
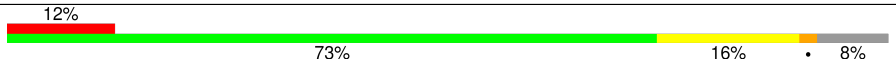
Mol	Chain	Length	Quality of chain
1	F	311	
1	G	311	
1	H	311	
1	I	311	
1	J	311	

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	GAL	A	4	-	-	X	-
2	BGC	A	5	-	-	X	-
2	FUC	D	1	-	-	-	X
2	GAL	D	4	-	-	X	-
2	BGC	D	5	-	-	X	-
2	FUC	D	534	-	-	X	X
2	FUC	E	1	-	-	-	X
2	GAL	E	533	-	-	X	-
2	BGC	E	534	-	-	X	-
2	GAL	G	535	-	-	X	-
2	BGC	G	536	-	-	X	-
3	FUC	B	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24066 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
			2404	1517	415	462	10			
1	B	308	Total	C	N	O	S	0	0	0
			2392	1510	411	461	10			
1	C	311	Total	C	N	O	S	0	0	0
			2403	1514	413	466	10			
1	D	307	Total	C	N	O	S	0	0	0
			2385	1507	410	458	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
			2383	1506	407	460	10			
1	H	292	Total	C	N	O	S	0	0	0
			2266	1441	385	431	9			
1	I	285	Total	C	N	O	S	0	0	0
			2184	1385	378	413	8			
1	J	307	Total	C	N	O	S	0	0	0
			2386	1507	410	459	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 (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	5	Total	C	N	O	0	0
			58	32	1	25		
2	D	5	Total	C	N	O	0	0
			58	32	1	25		
2	D	5	Total	C	N	O	0	0
			58	32	1	25		
2	E	5	Total	C	N	O	0	0
			58	32	1	25		
2	G	5	Total	C	N	O	0	0
			58	32	1	25		
2	G	5	Total	C	N	O	0	0
			58	32	1	25		
2	A	5	Total	C	N	O	0	0
			58	32	1	25		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	2	Total	C	O	0	0
			22	12	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

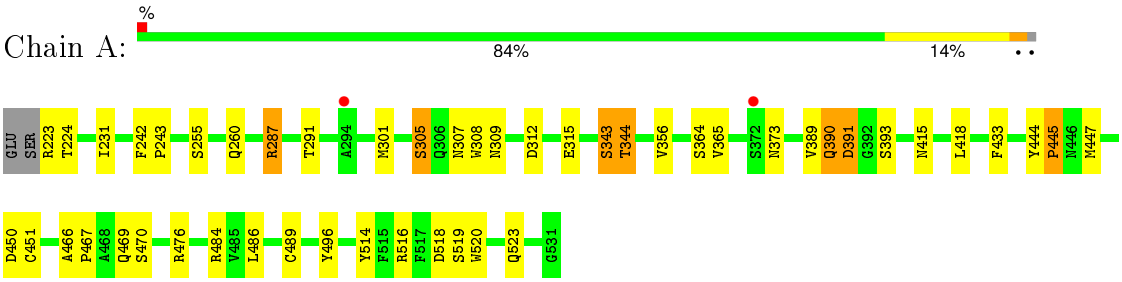
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	3	Total	C	N	O	0	0
			36	20	1	15		

3 Residue-property plots (i)

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.

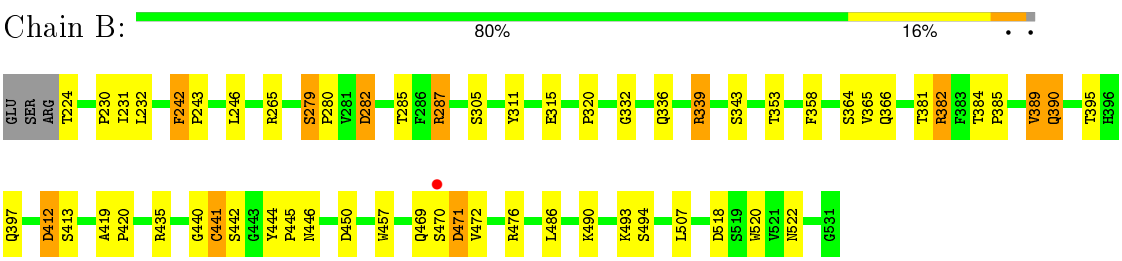
- Molecule 1: Capsid

Chain A:



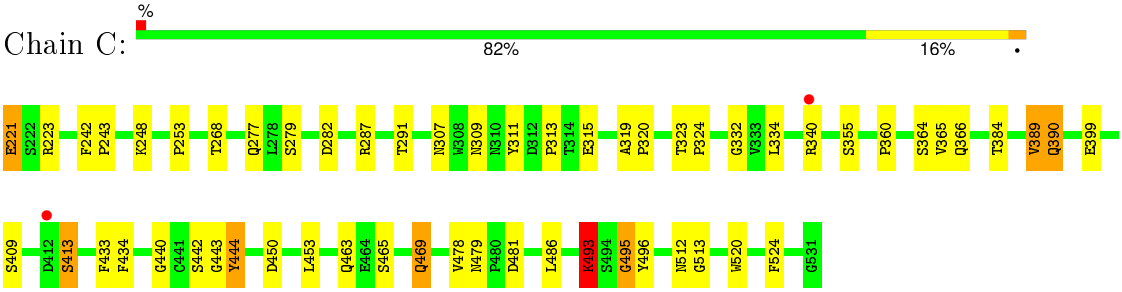
- Molecule 1: Capsid

Chain B:



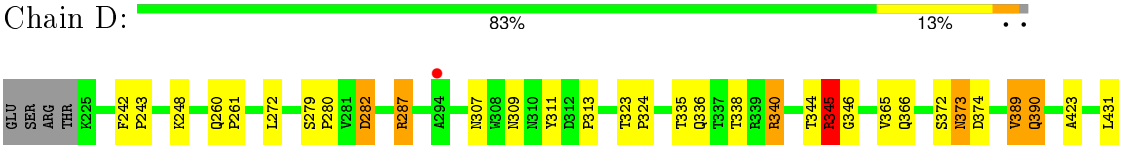
- Molecule 1: Capsid

Chain C:



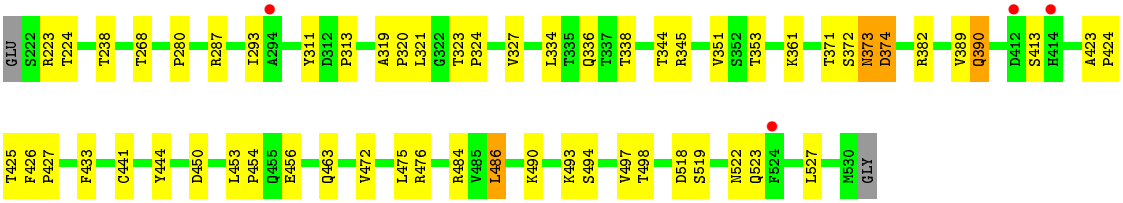
- Molecule 1: Capsid

Chain D:



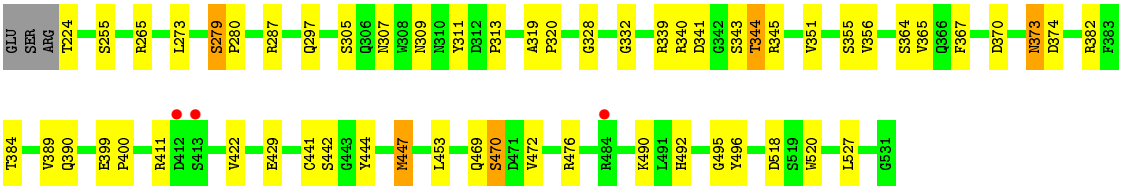
• Molecule 1: Capsid

Chain E:



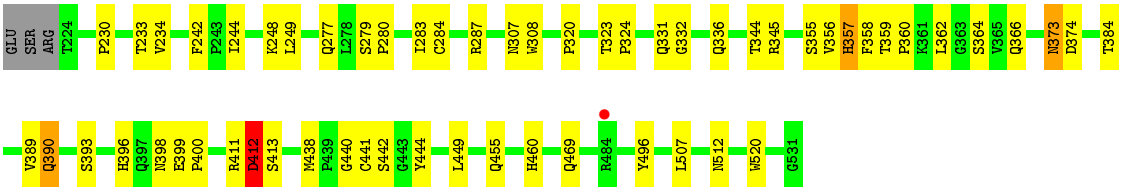
• Molecule 1: Capsid

Chain F:



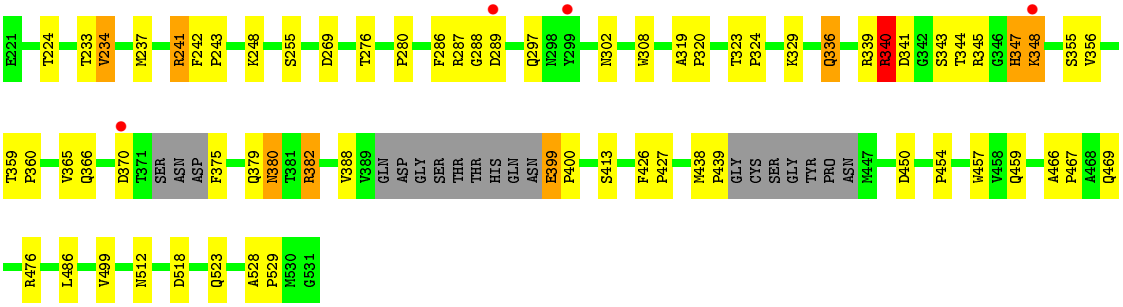
• Molecule 1: Capsid

Chain G:



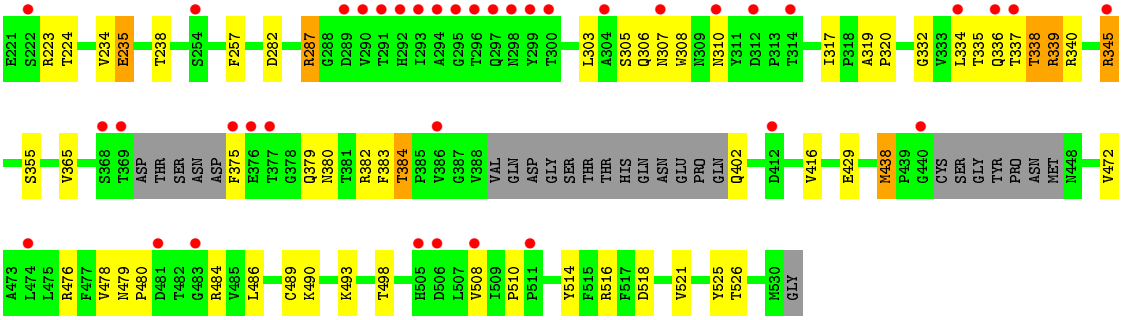
• Molecule 1: Capsid

Chain H:



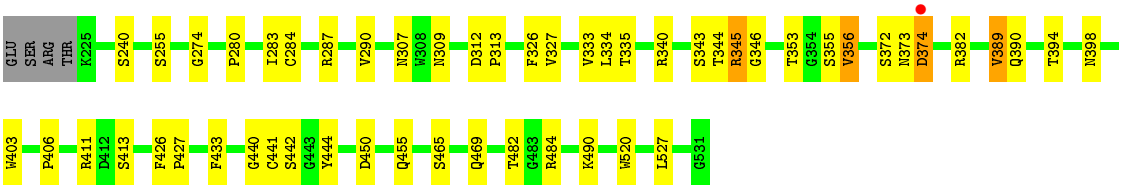
• Molecule 1: Capsid

Chain I:



- Molecule 1: Capsid

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	242.22Å 339.03Å 124.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 2.84 39.52 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.85-2.84) 99.2 (39.52-2.84)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.231 0.187 , 0.227	Depositor DCC
R_{free} test set	6014 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 25.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 119234 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.04	3/2474 (0.1%)	0.91	5/3385 (0.1%)
1	B	0.97	3/2462 (0.1%)	0.91	3/3369 (0.1%)
1	C	0.99	5/2472 (0.2%)	0.90	5/3384 (0.1%)
1	D	0.93	1/2455 (0.0%)	0.88	2/3360 (0.1%)
1	E	0.96	1/2476 (0.0%)	0.89	3/3388 (0.1%)
1	F	0.85	0/2463	0.91	5/3371 (0.1%)
1	G	0.87	0/2453	0.85	2/3359 (0.1%)
1	H	0.91	2/2330 (0.1%)	0.88	4/3186 (0.1%)
1	I	0.90	2/2245 (0.1%)	0.77	1/3071 (0.0%)
1	J	0.86	0/2456	0.83	0/3361
All	All	0.93	17/24286 (0.1%)	0.87	30/33234 (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	A	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	340	ARG	CB-CG	-8.15	1.30	1.52
1	H	340	ARG	CZ-NH1	-8.09	1.22	1.33
1	A	451	CYS	CB-SG	-6.12	1.71	1.82
1	B	518	ASP	CB-CG	6.02	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	GLU	CG-CD	6.00	1.60	1.51
1	I	525	TYR	CA-CB	5.81	1.66	1.53
1	I	525	TYR	CD1-CE1	5.76	1.48	1.39
1	A	489	CYS	CB-SG	-5.72	1.72	1.81
1	B	441	CYS	CB-SG	-5.71	1.72	1.81
1	C	221	GLU	CB-CG	5.66	1.62	1.52
1	A	315	GLU	CG-CD	5.55	1.60	1.51
1	C	315	GLU	CG-CD	5.50	1.60	1.51
1	E	441	CYS	CB-SG	-5.28	1.73	1.81
1	C	434	PHE	CE2-CZ	5.22	1.47	1.37
1	C	221	GLU	CG-CD	5.16	1.59	1.51
1	D	423	ALA	CA-CB	-5.16	1.41	1.52
1	C	524	PHE	CA-CB	5.02	1.65	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	241	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	496	TYR	N-CA-CB	-7.74	96.66	110.60
1	F	496	TYR	N-CA-CB	-7.01	97.99	110.60
1	A	496	TYR	N-CA-CB	-6.99	98.02	110.60
1	F	345	ARG	N-CA-CB	-6.95	98.08	110.60
1	B	382	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	E	486	LEU	CA-CB-CG	-6.38	100.62	115.30
1	H	340	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	F	344	THR	CB-CA-C	-6.17	94.93	111.60
1	G	496	TYR	N-CA-CB	-6.04	99.72	110.60
1	A	301	MET	CG-SD-CE	5.94	109.70	100.20
1	A	391	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	F	344	THR	N-CA-C	5.72	126.45	111.00
1	D	374	ASP	N-CA-C	5.66	126.28	111.00
1	B	265	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	E	475	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	H	241	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	463	GLN	CB-CA-C	-5.31	99.78	110.40
1	C	334	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	312	ASP	CB-CG-OD1	5.29	123.06	118.30
1	G	374	ASP	N-CA-C	5.27	125.22	111.00
1	E	361	LYS	CD-CE-NZ	5.26	123.79	111.70
1	I	223	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	H	269	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	495	GLY	N-CA-C	5.16	125.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	493	LYS	CD-CE-NZ	-5.14	99.88	111.70
1	B	242	PHE	C-N-CD	5.14	139.19	128.40
1	A	523	GLN	CB-CA-C	-5.04	100.32	110.40
1	F	382	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	D	431	LEU	CB-CG-CD2	-5.01	102.49	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	SER	Peptide
1	D	345	ARG	Sidechain
1	E	223	ARG	Sidechain
1	H	336	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2404	0	2295	36	0
1	B	2392	0	2278	44	0
1	C	2403	0	2282	38	0
1	D	2385	0	2272	46	0
1	E	2406	0	2297	31	0
1	F	2393	0	2282	50	0
1	G	2383	0	2265	40	0
1	H	2266	0	2169	55	0
1	I	2184	0	2068	41	0
1	J	2386	0	2275	40	0
2	A	58	0	51	12	0
2	C	58	0	51	3	0
2	D	116	0	102	27	1
2	E	58	0	51	9	0
2	G	116	0	102	22	0
3	B	22	0	20	2	0
4	E	36	0	31	5	0
All	All	24066	0	22891	458	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (458) 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:A:4:GAL:H1	2:A:5:BGC:C6	1.60	1.23
2:D:4:GAL:H1	2:D:5:BGC:C6	1.60	1.18
1:G:411:ARG:O	1:G:412:ASP:HB3	1.45	1.17
2:G:2:GAL:O1	2:G:1:FUC:H5	1.44	1.16
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.01	1.15
1:H:382:ARG:CG	1:H:382:ARG:HH11	1.60	1.12
1:H:382:ARG:HG2	1:H:382:ARG:NH1	1.54	1.08
2:D:4:GAL:C1	2:D:5:BGC:C6	2.30	1.08
2:A:4:GAL:C1	2:A:5:BGC:C6	2.30	1.08
2:A:4:GAL:C1	2:A:5:BGC:H6C2	1.84	1.07
2:D:4:GAL:C1	2:D:5:BGC:H6C2	1.84	1.04
1:B:470:SER:HB2	1:B:520:TRP:HB3	1.39	1.04
1:H:339:ARG:HH11	1:H:345:ARG:CB	1.70	1.03
2:E:533:GAL:C1	2:E:534:BGC:H6C1	1.91	1.00
1:A:223:ARG:HG2	1:A:224:THR:H	1.26	1.00
1:D:443:GLY:HA2	2:D:534:FUC:C6	1.92	1.00
2:A:4:GAL:H1	2:A:5:BGC:H6C2	1.01	1.00
1:D:443:GLY:HA2	2:D:534:FUC:H61	1.44	0.99
2:D:4:GAL:H1	2:D:5:BGC:H6C2	1.01	0.98
2:C:3:NAG:O5	2:C:4:GAL:H4	1.61	0.98
1:H:339:ARG:NH1	1:H:345:ARG:CB	2.28	0.96
2:E:532:NAG:O5	2:E:533:GAL:H4	1.64	0.96
1:D:443:GLY:CA	2:D:534:FUC:H63	1.99	0.92
1:H:347:HIS:CD2	1:H:347:HIS:N	2.34	0.92
1:F:373:ASN:H	1:F:373:ASN:HD22	0.99	0.92
1:B:470:SER:CB	1:B:520:TRP:HB3	2.00	0.90
1:F:373:ASN:H	1:F:373:ASN:ND2	1.70	0.90
2:E:533:GAL:C1	2:E:534:BGC:C6	2.50	0.90
2:E:533:GAL:H1	2:E:534:BGC:C6	1.90	0.89
1:F:390:GLN:HG2	1:F:444:TYR:C	1.91	0.89
1:B:339:ARG:HG3	1:B:339:ARG:NH1	1.81	0.88
1:I:336:GLN:HG2	1:I:337:THR:H	1.39	0.87
1:H:382:ARG:HG2	1:H:382:ARG:HH11	0.71	0.85
1:F:469:GLN:HB2	1:F:520:TRP:CG	2.11	0.85
1:D:443:GLY:CA	2:D:534:FUC:C6	2.55	0.83
2:E:533:GAL:O5	2:E:534:BGC:H6C1	1.78	0.83
1:F:373:ASN:HD22	1:F:373:ASN:N	1.69	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:336:GLN:CG	1:I:337:THR:H	1.93	0.80
4:E:4:GAL:O2	4:E:5:BGC:C6	2.30	0.80
1:I:339:ARG:HD2	1:I:345:ARG:NH1	1.97	0.80
1:H:347:HIS:HD2	1:H:347:HIS:N	1.77	0.80
2:E:532:NAG:O5	2:E:533:GAL:C4	2.30	0.80
1:H:347:HIS:H	1:H:347:HIS:CD2	1.95	0.79
1:A:223:ARG:HG2	1:A:224:THR:N	1.98	0.78
1:B:412:ASP:OD2	1:J:394:THR:HG23	1.84	0.78
1:A:307:ASN:O	1:A:308:TRP:HB2	1.83	0.77
2:D:3:NAG:N2	2:D:2:GAL:H1	1.99	0.77
1:H:382:ARG:NH1	1:H:382:ARG:CG	2.30	0.77
2:A:4:GAL:H5	2:A:5:BGC:H6C2	1.66	0.76
1:C:469:GLN:HG3	1:C:520:TRP:CD1	2.20	0.75
2:C:3:NAG:O5	2:C:4:GAL:C4	2.33	0.75
2:A:3:NAG:N2	2:A:2:GAL:H1	1.99	0.75
2:G:2:GAL:O1	2:G:1:FUC:C5	2.30	0.75
2:D:4:GAL:H5	2:D:5:BGC:H6C2	1.66	0.75
1:F:469:GLN:HB2	1:F:520:TRP:CD2	2.21	0.75
4:E:4:GAL:O2	4:E:5:BGC:H6C2	1.86	0.75
1:G:469:GLN:HB2	1:G:520:TRP:CD1	2.22	0.74
1:G:390:GLN:CG	1:G:444:TYR:H	2.01	0.74
1:H:438:MET:HG3	1:H:439:PRO:HD2	1.69	0.74
1:H:297:GLN:NE2	1:H:370:ASP:O	2.20	0.74
1:F:373:ASN:ND2	1:F:373:ASN:N	2.31	0.74
1:G:441:CYS:O	1:J:346:GLY:N	2.21	0.73
1:C:481:ASP:CG	1:C:512:ASN:HD21	1.90	0.73
1:F:390:GLN:HE21	1:F:444:TYR:H	1.37	0.73
1:I:334:LEU:CD1	1:I:383:PHE:HB2	2.18	0.73
1:A:223:ARG:CG	1:A:224:THR:H	2.00	0.73
1:A:231:ILE:O	1:A:231:ILE:HG22	1.87	0.73
2:G:535:GAL:O6	2:G:536:BGC:H6C2	1.89	0.73
1:J:345:ARG:HD3	1:J:374:ASP:OD1	1.89	0.72
1:H:339:ARG:HB2	1:H:343:SER:O	1.88	0.72
1:A:343:SER:HB3	1:C:444:TYR:CE1	2.24	0.72
1:I:282:ASP:OD2	1:I:306:GLN:NE2	2.22	0.71
1:I:336:GLN:HB2	1:I:380:ASN:O	1.90	0.71
2:D:532:NAG:O5	2:D:535:GAL:H4	1.90	0.71
1:D:470:SER:OG	1:D:520:TRP:HB3	1.89	0.71
1:G:412:ASP:OD1	1:G:412:ASP:C	2.29	0.70
1:B:287:ARG:HH11	1:B:287:ARG:HB2	1.56	0.70
1:A:390:GLN:HG2	1:A:444:TYR:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:THR:HG22	1:H:324:PRO:HD2	1.74	0.69
1:D:390:GLN:HG2	1:D:444:TYR:C	2.11	0.69
1:I:336:GLN:CG	1:I:337:THR:N	2.54	0.69
1:C:453:LEU:HD21	1:C:495:GLY:O	1.92	0.69
1:D:390:GLN:HG3	1:D:444:TYR:H	1.57	0.69
1:E:338:THR:HG23	1:E:345:ARG:HH22	1.57	0.69
1:F:390:GLN:HG2	1:F:444:TYR:O	1.92	0.68
2:G:535:GAL:O5	2:G:536:BGC:H6C2	1.92	0.68
1:F:469:GLN:HB2	1:F:520:TRP:CD1	2.28	0.68
1:A:344:THR:HG22	1:C:442:SER:N	2.09	0.68
1:J:307:ASN:HD21	1:J:309:ASN:HB2	1.59	0.68
1:I:480:PRO:HB3	1:I:514:TYR:HE2	1.58	0.68
1:C:253:PRO:HG3	4:E:5:BGC:H1	1.76	0.68
1:D:442:SER:HA	1:F:344:THR:O	1.94	0.68
1:G:469:GLN:HB2	1:G:520:TRP:CG	2.28	0.68
1:C:311:TYR:O	1:C:313:PRO:HD3	1.94	0.68
1:D:336:GLN:HB3	1:D:345:ARG:HH21	1.59	0.67
1:D:338:THR:OG1	1:D:345:ARG:NH1	2.24	0.67
1:F:472:VAL:HG11	1:F:490:LYS:HD3	1.75	0.67
2:G:532:NAG:N2	2:G:533:GAL:H1	2.09	0.66
1:I:476:ARG:HD3	1:I:518:ASP:OD2	1.95	0.66
2:G:535:GAL:O5	2:G:536:BGC:C5	2.42	0.66
1:B:343:SER:HB2	3:B:1:FUC:H63	1.78	0.65
1:J:373:ASN:N	1:J:373:ASN:OD1	2.29	0.65
1:H:336:GLN:HE21	1:H:379:GLN:HB2	1.61	0.65
1:H:336:GLN:OE1	1:H:375:PHE:HD1	1.80	0.65
2:A:4:GAL:C1	2:A:5:BGC:H6C1	2.26	0.65
1:E:373:ASN:N	1:E:373:ASN:OD1	2.29	0.65
1:H:286:PHE:CZ	1:H:323:THR:HG23	2.32	0.65
1:I:472:VAL:HG11	1:I:490:LYS:HD3	1.80	0.65
2:G:535:GAL:O5	2:G:536:BGC:C6	2.45	0.64
1:D:389:VAL:HG22	1:D:442:SER:HB3	1.78	0.64
4:E:4:GAL:O2	4:E:5:BGC:H6C1	1.97	0.64
1:D:373:ASN:N	1:D:373:ASN:OD1	2.30	0.64
1:G:373:ASN:OD1	1:G:373:ASN:N	2.30	0.64
1:A:287:ARG:HB2	1:A:287:ARG:HH11	1.62	0.64
1:B:412:ASP:OD2	1:J:394:THR:CG2	2.46	0.64
1:C:469:GLN:CG	1:C:520:TRP:CD1	2.81	0.64
1:D:443:GLY:N	2:D:534:FUC:H63	2.13	0.64
1:J:390:GLN:HG2	1:J:444:TYR:C	2.18	0.64
1:H:344:THR:OG1	1:H:345:ARG:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:532:NAG:O5	2:G:535:GAL:H4	1.99	0.63
1:I:340:ARG:HD2	1:J:274:GLY:O	1.98	0.63
1:F:469:GLN:HA	1:F:469:GLN:OE1	1.98	0.63
1:H:286:PHE:CE1	1:H:323:THR:HG23	2.33	0.63
1:J:307:ASN:ND2	1:J:309:ASN:HB2	2.14	0.63
1:A:260:GLN:HG2	1:A:260:GLN:O	1.99	0.63
2:D:4:GAL:C1	2:D:5:BGC:H6C1	2.26	0.62
1:D:390:GLN:CG	1:D:444:TYR:H	2.12	0.62
1:G:390:GLN:HG2	1:G:444:TYR:C	2.19	0.62
1:H:476:ARG:HD3	1:H:518:ASP:OD2	1.99	0.62
1:B:390:GLN:HG2	1:B:444:TYR:C	2.20	0.62
1:G:390:GLN:HG3	1:G:444:TYR:H	1.64	0.61
2:A:4:GAL:H5	2:A:5:BGC:C6	2.31	0.61
1:G:390:GLN:HG2	1:G:444:TYR:H	1.64	0.61
1:D:390:GLN:HG2	1:D:445:PRO:N	2.15	0.61
2:D:4:GAL:H5	2:D:5:BGC:C6	2.31	0.61
1:J:394:THR:HG22	1:J:398:ASN:ND2	2.16	0.61
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.81	0.61
1:B:472:VAL:HG11	1:B:490:LYS:HD3	1.83	0.61
1:F:390:GLN:HG3	1:F:444:TYR:H	1.66	0.61
1:D:390:GLN:O	1:D:443:GLY:HA3	2.01	0.60
1:A:344:THR:HG23	1:C:440:GLY:C	2.22	0.60
3:B:2:GAL:H1	4:E:3:NAG:N2	2.17	0.60
1:C:479:ASN:OD1	1:C:481:ASP:HB2	2.02	0.60
1:D:440:GLY:HA3	1:F:344:THR:HG21	1.83	0.60
1:B:242:PHE:CD2	1:B:243:PRO:HD2	2.36	0.60
1:D:390:GLN:HG3	1:D:444:TYR:N	2.17	0.60
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.36	0.60
1:D:307:ASN:OD1	1:D:309:ASN:HB2	2.01	0.59
1:J:490:LYS:HG3	1:J:527:LEU:HD11	1.85	0.59
1:G:412:ASP:OD1	1:G:413:SER:HB2	2.03	0.59
1:I:334:LEU:HA	1:I:382:ARG:O	2.03	0.58
2:D:532:NAG:O5	2:D:535:GAL:C4	2.49	0.58
1:F:429:GLU:OE2	1:F:490:LYS:HE3	2.03	0.58
1:C:223:ARG:NH2	1:H:276:THR:O	2.30	0.58
1:J:433:PHE:HB3	1:J:450:ASP:HB3	1.84	0.58
1:B:471:ASP:HA	1:B:493:LYS:HD3	1.85	0.57
1:B:435:ARG:HB2	1:B:450:ASP:OD1	2.05	0.57
1:H:380:ASN:N	1:H:380:ASN:OD1	2.36	0.57
1:J:389:VAL:HG22	1:J:442:SER:HB3	1.86	0.56
1:F:469:GLN:CB	1:F:520:TRP:CD1	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:532:NAG:H2	2:G:534:FUC:H5	1.86	0.56
1:H:336:GLN:NE2	1:H:379:GLN:HB2	2.21	0.56
1:H:347:HIS:H	1:H:347:HIS:HD2	1.40	0.56
1:I:336:GLN:HG2	1:I:337:THR:N	2.16	0.56
1:C:268:THR:HG23	1:C:493:LYS:HA	1.88	0.56
1:F:389:VAL:HG22	1:F:442:SER:HB3	1.88	0.56
1:B:231:ILE:HG22	1:B:231:ILE:O	2.06	0.56
1:A:287:ARG:HB2	1:A:287:ARG:NH1	2.21	0.56
1:I:317:ILE:HD12	1:I:319:ALA:O	2.06	0.56
1:E:472:VAL:HG11	1:E:490:LYS:HD3	1.89	0.55
1:B:470:SER:OG	1:B:520:TRP:HB3	2.06	0.55
2:D:4:GAL:C5	2:D:5:BGC:H6C2	2.34	0.55
1:E:268:THR:HG23	1:E:493:LYS:HA	1.88	0.55
1:C:242:PHE:CD2	1:C:243:PRO:HD2	2.41	0.55
1:I:334:LEU:HD12	1:I:383:PHE:CA	2.38	0.54
1:J:327:VAL:HA	1:J:353:THR:OG1	2.08	0.54
1:H:438:MET:HG3	1:H:439:PRO:CD	2.37	0.54
1:H:365:VAL:CG1	1:H:366:GLN:N	2.70	0.54
2:G:2:GAL:C1	2:G:1:FUC:H5	2.35	0.54
1:F:390:GLN:HE21	1:F:444:TYR:N	2.03	0.54
1:J:389:VAL:HG23	1:J:441:CYS:HB2	1.90	0.54
1:C:444:TYR:CD2	1:C:444:TYR:N	2.76	0.54
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.43	0.54
2:G:535:GAL:O6	2:G:536:BGC:C6	2.55	0.54
1:A:518:ASP:OD2	1:A:519:SER:OG	2.25	0.54
1:A:444:TYR:CD2	1:A:444:TYR:N	2.76	0.53
1:A:390:GLN:CG	1:A:444:TYR:O	2.56	0.53
1:H:399:GLU:HB2	1:H:400:PRO:HA	1.88	0.53
1:I:334:LEU:HD13	1:I:383:PHE:HD1	1.73	0.53
1:D:469:GLN:HG3	1:D:520:TRP:CD1	2.43	0.53
2:G:534:FUC:H63	1:J:343:SER:HB2	1.91	0.53
1:A:390:GLN:HG2	1:A:445:PRO:HA	1.91	0.53
1:G:359:THR:O	1:G:360:PRO:C	2.44	0.53
2:A:4:GAL:C5	2:A:5:BGC:H6C2	2.34	0.53
1:G:280:PRO:HB3	1:G:455:GLN:HG2	1.90	0.53
1:D:287:ARG:HB2	1:D:287:ARG:HH11	1.73	0.53
1:B:389:VAL:HG23	1:B:441:CYS:HB2	1.90	0.53
1:D:443:GLY:N	2:D:534:FUC:C6	2.72	0.53
1:B:279:SER:HB3	1:B:282:ASP:HB2	1.91	0.52
1:D:443:GLY:C	2:D:534:FUC:H63	2.30	0.52
1:E:371:THR:HG21	1:E:374:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:469:GLN:CG	1:F:520:TRP:CD1	2.92	0.52
1:D:287:ARG:NH1	1:D:287:ARG:HB2	2.24	0.52
1:F:470:SER:HB2	1:F:520:TRP:HB3	1.92	0.52
1:B:469:GLN:HB2	1:B:520:TRP:CG	2.44	0.52
1:D:336:GLN:O	1:D:344:THR:HA	2.09	0.52
1:F:390:GLN:CG	1:F:444:TYR:H	2.22	0.52
1:F:469:GLN:HB2	1:F:520:TRP:CE2	2.44	0.52
1:I:334:LEU:HD12	1:I:383:PHE:HA	1.91	0.52
1:A:344:THR:HB	1:C:443:GLY:O	2.10	0.51
1:B:232:LEU:HG	1:E:463:GLN:HE22	1.75	0.51
1:E:238:THR:N	1:E:456:GLU:OE1	2.39	0.51
1:G:438:MET:CE	1:G:449:LEU:HB2	2.40	0.51
1:H:388:VAL:HG22	1:H:438:MET:HG2	1.92	0.51
1:F:328:GLY:HA3	1:F:400:PRO:HB3	1.91	0.51
1:J:394:THR:HG22	1:J:398:ASN:HD21	1.75	0.51
1:H:323:THR:HG22	1:H:324:PRO:CD	2.40	0.51
1:E:327:VAL:HA	1:E:353:THR:OG1	2.11	0.51
2:E:533:GAL:C5	2:E:534:BGC:H6C1	2.41	0.51
1:A:469:GLN:HB2	1:A:520:TRP:CG	2.47	0.50
1:H:348:LYS:HD3	1:H:370:ASP:OD2	2.11	0.50
1:F:469:GLN:HG3	1:F:520:TRP:CD1	2.46	0.50
1:F:374:ASP:OD1	1:F:374:ASP:O	2.30	0.50
1:I:489:CYS:HB2	1:I:498:THR:O	2.11	0.50
1:F:265:ARG:HB3	1:F:273:LEU:HB2	1.93	0.50
1:G:412:ASP:OD1	1:G:412:ASP:O	2.30	0.50
1:F:297:GLN:NE2	1:F:370:ASP:O	2.44	0.50
1:B:232:LEU:HG	1:E:463:GLN:NE2	2.27	0.50
1:H:242:PHE:CD2	1:H:243:PRO:HD2	2.47	0.50
1:J:356:VAL:HG23	1:J:411:ARG:HG3	1.94	0.50
1:E:351:VAL:O	1:E:351:VAL:HG13	2.12	0.49
1:B:390:GLN:CG	1:B:444:TYR:H	2.26	0.49
1:H:528:ALA:O	1:H:529:PRO:C	2.50	0.49
1:G:323:THR:HG23	1:G:324:PRO:HD2	1.93	0.49
1:A:445:PRO:O	1:A:447:MET:HG3	2.12	0.49
1:A:344:THR:CG2	1:C:442:SER:N	2.73	0.49
1:B:230:PRO:HD2	1:B:457:TRP:NE1	2.27	0.49
1:I:287:ARG:HB2	1:I:287:ARG:HH11	1.78	0.49
1:D:443:GLY:H	2:D:534:FUC:C6	2.25	0.49
2:G:532:NAG:O5	2:G:535:GAL:C4	2.61	0.49
1:I:319:ALA:HB1	1:I:320:PRO:HD2	1.94	0.48
1:E:268:THR:CG2	1:E:493:LYS:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLN:HG3	1:B:381:THR:OG1	2.13	0.48
1:D:390:GLN:CG	1:D:444:TYR:N	2.74	0.48
1:F:490:LYS:HG3	1:F:527:LEU:HD11	1.95	0.48
1:A:223:ARG:HB2	1:A:223:ARG:HH11	1.78	0.48
1:B:339:ARG:CG	1:B:339:ARG:HH11	1.94	0.48
1:B:507:LEU:N	1:B:507:LEU:HD12	2.29	0.48
2:G:532:NAG:HN2	2:G:533:GAL:H1	1.78	0.48
1:G:230:PRO:HG3	1:G:460:HIS:HB2	1.96	0.48
1:E:338:THR:CG2	1:E:345:ARG:HH12	2.26	0.48
1:A:514:TYR:OH	1:A:516:ARG:NH2	2.47	0.48
1:E:423:ALA:O	1:E:425:THR:HG23	2.13	0.48
1:J:482:THR:OG1	1:J:484:ARG:HB2	2.14	0.48
1:H:233:THR:HG21	1:H:512:ASN:HA	1.96	0.48
1:J:283:ILE:O	1:J:284:CYS:HB2	2.14	0.48
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.49	0.48
1:I:338:THR:O	1:I:338:THR:OG1	2.30	0.47
1:A:242:PHE:CD2	1:A:243:PRO:HD2	2.48	0.47
1:C:307:ASN:OD1	1:C:309:ASN:HB2	2.14	0.47
1:C:389:VAL:HG22	1:C:442:SER:HB3	1.95	0.47
1:D:340:ARG:HB3	1:D:340:ARG:HE	1.47	0.47
1:J:280:PRO:HB3	1:J:455:GLN:HG2	1.95	0.47
1:E:433:PHE:HB3	1:E:450:ASP:HB3	1.96	0.47
1:F:453:LEU:HG	1:F:495:GLY:O	2.13	0.47
1:G:411:ARG:O	1:G:412:ASP:CB	2.30	0.47
1:C:320:PRO:HD2	1:C:360:PRO:HB2	1.96	0.47
1:A:305:SER:HB2	1:A:309:ASN:O	2.13	0.47
1:A:307:ASN:O	1:A:308:TRP:CB	2.58	0.47
1:B:285:THR:HG22	1:B:385:PRO:CD	2.44	0.47
1:F:341:ASP:HB2	1:F:343:SER:H	1.79	0.47
1:C:453:LEU:CD2	1:C:495:GLY:O	2.62	0.47
1:F:469:GLN:CB	1:F:520:TRP:CG	2.90	0.47
1:D:442:SER:CA	1:F:344:THR:O	2.60	0.47
1:C:323:THR:HG23	1:C:324:PRO:HD2	1.97	0.47
1:B:280:PRO:HG2	1:E:280:PRO:HG2	1.97	0.47
1:E:390:GLN:HG3	1:E:444:TYR:H	1.80	0.47
1:C:242:PHE:CG	1:C:243:PRO:HD2	2.49	0.46
1:D:490:LYS:HG3	1:D:527:LEU:HD11	1.96	0.46
1:G:356:VAL:C	1:G:358:PHE:H	2.18	0.46
1:D:279:SER:HB3	1:D:282:ASP:HB2	1.97	0.46
1:H:319:ALA:HB1	1:H:320:PRO:HD2	1.97	0.46
1:D:346:GLY:N	1:F:441:CYS:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4:GAL:C5	2:A:5:BGC:C6	2.92	0.46
1:E:323:THR:HG23	1:E:324:PRO:HD2	1.97	0.46
1:F:311:TYR:O	1:F:313:PRO:HD3	2.15	0.46
1:A:223:ARG:NH1	1:A:223:ARG:HB2	2.29	0.46
1:G:332:GLY:HA3	1:G:384:THR:O	2.15	0.46
1:C:365:VAL:CG1	1:C:366:GLN:N	2.77	0.46
1:J:403:TRP:CE3	1:J:403:TRP:HA	2.49	0.46
1:F:351:VAL:HB	1:F:367:PHE:CE1	2.51	0.46
1:I:334:LEU:HD12	1:I:383:PHE:HB2	1.96	0.46
1:E:497:VAL:HG12	1:E:498:THR:N	2.31	0.46
1:F:390:GLN:NE2	1:F:444:TYR:H	2.08	0.46
1:I:429:GLU:OE2	1:I:490:LYS:HE3	2.16	0.46
1:H:365:VAL:HG12	1:H:366:GLN:N	2.30	0.46
1:I:319:ALA:HB1	1:I:320:PRO:CD	2.45	0.46
2:G:4:GAL:H1	2:G:5:BGC:H5	1.25	0.45
1:I:334:LEU:HD12	1:I:383:PHE:CB	2.47	0.45
2:D:4:GAL:C5	2:D:5:BGC:C6	2.92	0.45
2:D:4:GAL:O5	2:D:5:BGC:H6C1	2.17	0.45
1:D:311:TYR:O	1:D:313:PRO:HD3	2.17	0.45
1:G:242:PHE:O	1:G:244:ILE:N	2.49	0.45
1:D:242:PHE:CD2	1:D:243:PRO:HD2	2.51	0.45
1:E:311:TYR:O	1:E:313:PRO:HD3	2.17	0.45
1:A:391:ASP:C	1:A:391:ASP:OD1	2.55	0.45
1:F:332:GLY:HA3	1:F:384:THR:O	2.16	0.45
1:H:339:ARG:NH1	1:H:345:ARG:O	2.50	0.45
1:F:399:GLU:HB2	1:F:400:PRO:HA	1.99	0.45
1:J:326:PHE:O	1:J:406:PRO:HG3	2.17	0.45
1:B:440:GLY:HA3	1:E:344:THR:HG21	1.99	0.45
1:H:280:PRO:HD3	1:H:459:GLN:HE22	1.82	0.45
2:G:534:FUC:O3	1:J:345:ARG:HG3	2.17	0.45
1:E:338:THR:CG2	1:E:345:ARG:HH22	2.27	0.45
1:B:230:PRO:HD2	1:B:457:TRP:CD1	2.52	0.45
1:B:470:SER:HB2	1:B:520:TRP:CB	2.27	0.44
1:F:390:GLN:HG3	1:F:444:TYR:N	2.32	0.44
1:I:336:GLN:HG3	1:I:337:THR:HG23	1.98	0.44
2:A:4:GAL:O5	2:A:5:BGC:H6C1	2.17	0.44
1:G:389:VAL:HG23	1:G:441:CYS:HB2	1.99	0.44
2:C:4:GAL:H1	2:C:5:BGC:H5	1.91	0.44
1:H:323:THR:CG2	1:H:324:PRO:HD2	2.43	0.44
1:D:389:VAL:HG23	1:D:441:CYS:HB2	2.00	0.44
1:F:307:ASN:HD21	1:F:309:ASN:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:SER:HG	2:E:2:GAL:HO3	1.63	0.44
2:D:533:GAL:O1	2:D:534:FUC:H5	2.18	0.44
1:G:331:GLN:HB3	1:G:441:CYS:SG	2.58	0.44
2:D:535:GAL:H1	2:D:536:BGC:H5	1.44	0.44
1:J:390:GLN:HG3	1:J:444:TYR:H	1.83	0.44
1:J:240:SER:O	1:J:283:ILE:HD13	2.16	0.44
1:I:332:GLY:HA3	1:I:384:THR:O	2.18	0.44
1:E:321:LEU:HD23	1:E:321:LEU:HA	1.64	0.44
1:H:287:ARG:HB3	1:H:308:TRP:CZ3	2.52	0.44
2:G:2:GAL:C2	2:G:1:FUC:H5	2.46	0.44
1:H:280:PRO:HD3	1:H:459:GLN:NE2	2.33	0.44
1:D:433:PHE:HB3	1:D:450:ASP:HB3	2.00	0.44
1:G:307:ASN:O	1:G:308:TRP:HB2	2.17	0.44
1:J:394:THR:CG2	1:J:398:ASN:HD21	2.31	0.44
1:E:336:GLN:OE1	1:E:345:ARG:NH1	2.50	0.44
1:D:323:THR:HG23	1:D:324:PRO:HD2	2.00	0.44
1:H:359:THR:N	1:H:360:PRO:CD	2.81	0.44
1:E:518:ASP:O	1:E:519:SER:HB3	2.17	0.44
1:E:426:PHE:CD2	1:E:427:PRO:HD2	2.53	0.44
1:F:492:HIS:N	1:F:492:HIS:CD2	2.86	0.44
1:J:469:GLN:HG3	1:J:520:TRP:CD1	2.52	0.44
1:F:279:SER:HA	1:F:280:PRO:HD3	1.74	0.44
2:E:533:GAL:H1	2:E:534:BGC:H5	1.46	0.44
2:G:535:GAL:H1	2:G:536:BGC:H5	1.45	0.44
1:D:389:VAL:HG22	1:D:442:SER:CB	2.45	0.44
1:G:277:GLN:OE1	1:G:279:SER:HB3	2.17	0.44
1:J:390:GLN:HE21	1:J:444:TYR:H	1.66	0.44
1:I:340:ARG:CD	1:J:274:GLY:O	2.65	0.44
1:B:246:LEU:HA	1:B:246:LEU:HD23	1.81	0.44
1:E:484:ARG:HG3	1:E:484:ARG:HH11	1.83	0.44
1:I:235:GLU:HG2	1:I:235:GLU:H	1.41	0.43
1:A:415:ASN:HB3	1:A:418:LEU:HD21	1.99	0.43
1:H:339:ARG:O	1:H:341:ASP:N	2.51	0.43
1:I:334:LEU:CD1	1:I:383:PHE:CB	2.94	0.43
1:J:335:THR:HA	1:J:345:ARG:O	2.18	0.43
1:I:303:LEU:HD13	1:I:320:PRO:HG2	1.99	0.43
1:C:332:GLY:HA3	1:C:384:THR:O	2.19	0.43
1:D:280:PRO:HG3	1:F:280:PRO:HG2	2.00	0.43
1:D:476:ARG:N	1:D:476:ARG:HD2	2.31	0.43
1:C:453:LEU:CG	1:C:495:GLY:O	2.66	0.43
1:J:482:THR:OG1	1:J:484:ARG:N	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:VAL:CG1	1:D:366:GLN:N	2.81	0.43
1:I:438:MET:HB3	1:I:438:MET:HE3	1.92	0.43
1:B:332:GLY:HA3	1:B:384:THR:O	2.17	0.43
1:D:476:ARG:HD3	1:D:518:ASP:OD2	2.18	0.43
1:D:272:LEU:HB2	1:H:340:ARG:NH2	2.33	0.43
1:G:249:LEU:HB2	1:G:507:LEU:HB2	2.00	0.43
1:B:353:THR:HG22	1:B:358:PHE:CE1	2.54	0.43
1:C:319:ALA:HB1	1:C:320:PRO:HD2	2.01	0.43
1:G:344:THR:HG21	1:J:440:GLY:HA3	1.99	0.43
1:C:279:SER:HB3	1:C:282:ASP:HB2	2.01	0.43
1:H:234:VAL:HA	1:H:237:MET:HE2	2.01	0.43
1:A:344:THR:HG23	1:C:440:GLY:O	2.18	0.43
2:D:3:NAG:HN2	2:D:2:GAL:H1	1.82	0.42
1:D:335:THR:HA	1:D:345:ARG:O	2.19	0.42
1:G:336:GLN:O	1:G:344:THR:HA	2.19	0.42
1:J:312:ASP:HA	1:J:313:PRO:HD3	1.89	0.42
1:H:339:ARG:C	1:H:341:ASP:N	2.73	0.42
1:I:478:VAL:HG21	1:I:516:ARG:NH1	2.34	0.42
1:E:453:LEU:HA	1:E:454:PRO:HD3	1.92	0.42
1:A:343:SER:HB3	1:C:444:TYR:CZ	2.53	0.42
1:F:319:ALA:HB1	1:F:320:PRO:HD2	2.02	0.42
1:B:470:SER:O	1:B:520:TRP:CE3	2.73	0.42
1:H:469:GLN:HA	1:H:469:GLN:OE1	2.18	0.42
1:A:484:ARG:NH1	1:A:484:ARG:HG3	2.33	0.42
1:G:438:MET:HE1	1:G:449:LEU:HB2	2.01	0.42
1:J:469:GLN:CG	1:J:520:TRP:CD1	3.02	0.42
1:B:397:GLN:HB3	1:B:446:ASN:HB2	2.01	0.42
2:D:4:GAL:O5	2:D:5:BGC:C6	2.67	0.42
1:G:390:GLN:HG2	1:G:444:TYR:N	2.32	0.42
2:G:532:NAG:O7	2:G:534:FUC:H3	2.19	0.42
2:G:535:GAL:O5	2:G:536:BGC:H5	2.05	0.42
1:G:356:VAL:HG23	1:G:357:HIS:N	2.34	0.42
2:G:4:GAL:O5	2:G:5:BGC:H6C1	2.20	0.42
1:A:466:ALA:HA	1:A:467:PRO:HD3	1.76	0.42
1:G:233:THR:HG21	1:G:512:ASN:HA	2.01	0.42
1:I:334:LEU:HD11	1:I:383:PHE:HB2	1.98	0.42
1:A:344:THR:CG2	1:C:440:GLY:C	2.88	0.42
1:G:320:PRO:HD2	1:G:360:PRO:HB2	2.01	0.42
1:D:443:GLY:H	2:D:534:FUC:H63	1.84	0.42
1:E:490:LYS:HG3	1:E:527:LEU:HD21	2.02	0.42
1:C:478:VAL:O	1:C:513:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:SER:HB2	1:C:413:SER:HB3	2.02	0.42
2:G:534:FUC:H2	1:J:344:THR:O	2.19	0.41
1:H:323:THR:CG2	1:H:324:PRO:CD	2.98	0.41
1:G:359:THR:HB	1:G:362:LEU:HB2	2.02	0.41
1:F:307:ASN:ND2	1:F:309:ASN:HB2	2.35	0.41
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.84	0.41
1:A:433:PHE:HB3	1:A:450:ASP:HB3	2.02	0.41
1:H:426:PHE:CD2	1:H:427:PRO:HD2	2.54	0.41
1:I:338:THR:O	1:I:339:ARG:C	2.56	0.41
1:C:390:GLN:HB2	1:C:399:GLU:HG2	2.02	0.41
1:F:356:VAL:HG12	1:F:411:ARG:HG2	2.01	0.41
1:H:344:THR:H	1:H:344:THR:HG23	1.37	0.41
1:G:390:GLN:HB2	1:G:390:GLN:HE21	1.49	0.41
1:J:333:VAL:HG12	1:J:335:THR:HG22	2.00	0.41
1:I:306:GLN:C	1:I:308:TRP:H	2.24	0.41
1:F:476:ARG:HD3	1:F:518:ASP:OD2	2.20	0.41
1:E:423:ALA:HB1	1:E:424:PRO:HD2	2.03	0.41
1:B:419:ALA:HA	1:B:420:PRO:HD3	1.91	0.41
1:G:230:PRO:HG3	1:G:460:HIS:CB	2.49	0.41
1:I:307:ASN:O	1:I:308:TRP:HB2	2.21	0.41
1:H:454:PRO:HG2	1:H:457:TRP:CD1	2.56	0.41
1:B:365:VAL:CG1	1:B:366:GLN:N	2.83	0.41
1:G:399:GLU:HB2	1:G:400:PRO:HA	2.02	0.41
1:F:469:GLN:CA	1:F:469:GLN:OE1	2.68	0.41
1:C:365:VAL:HG13	1:C:366:GLN:N	2.36	0.41
1:C:277:GLN:OE1	1:C:279:SER:HB3	2.20	0.41
1:I:479:ASN:HB2	1:I:510:PRO:HG3	2.02	0.41
2:A:3:NAG:O5	2:A:4:GAL:H4	2.21	0.41
1:H:336:GLN:OE1	1:H:375:PHE:CD1	2.68	0.41
1:G:283:ILE:O	1:G:284:CYS:HB2	2.21	0.41
1:B:390:GLN:HG3	1:B:390:GLN:O	2.18	0.41
1:G:323:THR:CG2	1:G:324:PRO:HD2	2.50	0.41
1:H:466:ALA:HA	1:H:467:PRO:HD3	1.95	0.41
1:F:447:MET:HE2	1:F:447:MET:HB2	1.85	0.41
2:D:3:NAG:O5	2:D:4:GAL:H4	2.21	0.41
1:H:339:ARG:HD2	1:H:345:ARG:CB	2.51	0.41
1:I:336:GLN:OE1	1:I:375:PHE:HD1	2.03	0.41
1:I:336:GLN:HG3	1:I:337:THR:N	2.35	0.40
1:J:390:GLN:CG	1:J:444:TYR:H	2.35	0.40
1:J:426:PHE:HA	1:J:427:PRO:HD3	1.96	0.40
1:H:288:GLY:HA3	1:H:302:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:522:ASN:OD1	1:E:522:ASN:C	2.60	0.40
1:H:241:ARG:HD3	1:H:450:ASP:O	2.21	0.40
1:G:440:GLY:O	1:J:344:THR:HB	2.22	0.40
1:A:344:THR:CG2	1:C:442:SER:H	2.34	0.40
1:B:390:GLN:HG2	1:B:444:TYR:N	2.36	0.40
1:E:319:ALA:HB1	1:E:320:PRO:CD	2.50	0.40
1:I:337:THR:O	1:I:345:ARG:HB3	2.21	0.40
1:D:260:GLN:N	1:D:261:PRO:CD	2.85	0.40
1:C:453:LEU:HD11	1:C:495:GLY:O	2.21	0.40
1:B:390:GLN:HG2	1:B:445:PRO:N	2.36	0.40
1:H:224:THR:HG21	1:H:467:PRO:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:GAL:O2	2:D:5:BGC:O2[3_553]	1.29	0.91

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%)	295 (96%)	11 (4%)	1 (0%)	46 77
1	B	306/311 (98%)	296 (97%)	10 (3%)	0	100 100
1	C	309/311 (99%)	296 (96%)	13 (4%)	0	100 100
1	D	305/311 (98%)	290 (95%)	15 (5%)	0	100 100
1	E	307/311 (99%)	296 (96%)	11 (4%)	0	100 100
1	F	306/311 (98%)	294 (96%)	12 (4%)	0	100 100
1	G	306/311 (98%)	286 (94%)	18 (6%)	2 (1%)	26 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	284/311 (91%)	270 (95%)	14 (5%)	0	100 100
1	I	277/311 (89%)	258 (93%)	19 (7%)	0	100 100
1	J	305/311 (98%)	292 (96%)	13 (4%)	0	100 100
All	All	3012/3110 (97%)	2873 (95%)	136 (4%)	3 (0%)	56 86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	357	HIS
1	G	412	ASP
1	A	445	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/272 (99%)	255 (94%)	15 (6%)	26 57
1	B	269/272 (99%)	252 (94%)	17 (6%)	22 51
1	C	269/272 (99%)	254 (94%)	15 (6%)	26 57
1	D	267/272 (98%)	254 (95%)	13 (5%)	31 63
1	E	271/272 (100%)	256 (94%)	15 (6%)	27 58
1	F	269/272 (99%)	255 (95%)	14 (5%)	29 61
1	G	267/272 (98%)	253 (95%)	14 (5%)	29 61
1	H	253/272 (93%)	236 (93%)	17 (7%)	20 48
1	I	238/272 (88%)	213 (90%)	25 (10%)	8 23
1	J	268/272 (98%)	254 (95%)	14 (5%)	29 61
All	All	2641/2720 (97%)	2482 (94%)	159 (6%)	24 54

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	287	ARG
1	A	291	THR
1	A	305	SER
1	A	344	THR
1	A	356	VAL
1	A	364	SER
1	A	365	VAL
1	A	373	ASN
1	A	389	VAL
1	A	390	GLN
1	A	393	SER
1	A	470	SER
1	A	476	ARG
1	A	486	LEU
1	B	224	THR
1	B	279	SER
1	B	282	ASP
1	B	287	ARG
1	B	305	SER
1	B	339	ARG
1	B	364	SER
1	B	389	VAL
1	B	390	GLN
1	B	395	THR
1	B	412	ASP
1	B	413	SER
1	B	471	ASP
1	B	476	ARG
1	B	486	LEU
1	B	494	SER
1	B	522	ASN
1	C	221	GLU
1	C	248	LYS
1	C	287	ARG
1	C	291	THR
1	C	340	ARG
1	C	355	SER
1	C	364	SER
1	C	389	VAL
1	C	390	GLN
1	C	413	SER
1	C	444	TYR

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Mol	Chain	Res	Type
1	C	465	SER
1	C	469	GLN
1	C	486	LEU
1	C	493	LYS
1	D	248	LYS
1	D	282	ASP
1	D	287	ARG
1	D	340	ARG
1	D	345	ARG
1	D	372	SER
1	D	373	ASN
1	D	389	VAL
1	D	390	GLN
1	D	442	SER
1	D	476	ARG
1	D	494	SER
1	D	523	GLN
1	E	224	THR
1	E	287	ARG
1	E	293	ILE
1	E	334	LEU
1	E	372	SER
1	E	373	ASN
1	E	374	ASP
1	E	382	ARG
1	E	389	VAL
1	E	390	GLN
1	E	413	SER
1	E	476	ARG
1	E	486	LEU
1	E	494	SER
1	E	523	GLN
1	F	224	THR
1	F	255	SER
1	F	279	SER
1	F	287	ARG
1	F	305	SER
1	F	339	ARG
1	F	340	ARG
1	F	355	SER
1	F	364	SER
1	F	365	VAL

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Mol	Chain	Res	Type
1	F	373	ASN
1	F	422	VAL
1	F	447	MET
1	F	470	SER
1	G	234	VAL
1	G	248	LYS
1	G	287	ARG
1	G	345	ARG
1	G	355	SER
1	G	364	SER
1	G	366	GLN
1	G	373	ASN
1	G	390	GLN
1	G	393	SER
1	G	396	HIS
1	G	398	ASN
1	G	412	ASP
1	G	442	SER
1	H	234	VAL
1	H	248	LYS
1	H	255	SER
1	H	289	ASP
1	H	329	LYS
1	H	340	ARG
1	H	347	HIS
1	H	348	LYS
1	H	355	SER
1	H	356	VAL
1	H	380	ASN
1	H	382	ARG
1	H	399	GLU
1	H	413	SER
1	H	486	LEU
1	H	499	VAL
1	H	523	GLN
1	I	224	THR
1	I	234	VAL
1	I	235	GLU
1	I	238	THR
1	I	257	PHE
1	I	287	ARG
1	I	305	SER

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Mol	Chain	Res	Type
1	I	310	ASN
1	I	335	THR
1	I	338	THR
1	I	339	ARG
1	I	345	ARG
1	I	355	SER
1	I	365	VAL
1	I	379	GLN
1	I	384	THR
1	I	402	GLN
1	I	416	VAL
1	I	438	MET
1	I	484	ARG
1	I	486	LEU
1	I	493	LYS
1	I	508	VAL
1	I	521	VAL
1	I	526	THR
1	J	255	SER
1	J	287	ARG
1	J	290	VAL
1	J	334	LEU
1	J	340	ARG
1	J	345	ARG
1	J	355	SER
1	J	356	VAL
1	J	372	SER
1	J	374	ASP
1	J	382	ARG
1	J	389	VAL
1	J	413	SER
1	J	465	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	310	ASN
1	B	469	GLN
1	B	523	GLN
1	C	463	GLN
1	C	512	ASN

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Mol	Chain	Res	Type
1	D	390	GLN
1	D	505	HIS
1	E	309	ASN
1	E	523	GLN
1	F	297	GLN
1	F	373	ASN
1	F	390	GLN
1	F	523	GLN
1	G	390	GLN
1	G	492	HIS
1	H	347	HIS
1	H	523	GLN
1	I	331	GLN
1	J	292	HIS
1	J	390	GLN
1	J	523	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

40 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	A	1	2	10,10,11	0.43	0	14,14,16	1.04	1 (7%)
2	GAL	A	2	2	12,12,12	1.27	2 (16%)	17,17,17	2.44	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	3	2	14,14,15	1.99	3 (21%)	12,19,21	5.21	3 (25%)
2	GAL	A	4	2	11,11,12	0.97	0	12,15,17	2.54	4 (33%)
2	BGC	A	5	2	11,11,12	0.83	0	15,15,17	2.22	4 (26%)
3	FUC	B	1	3	10,10,11	0.43	0	14,14,16	1.01	1 (7%)
3	GAL	B	2	3,4	12,12,12	0.95	1 (8%)	17,17,17	1.81	5 (29%)
2	FUC	C	1	2	10,10,11	1.04	1 (10%)	14,14,16	2.56	3 (21%)
2	GAL	C	2	2	12,12,12	0.78	0	17,17,17	2.19	5 (29%)
2	NAG	C	3	2	14,14,15	0.68	0	12,19,21	4.37	2 (16%)
2	GAL	C	4	2	11,11,12	0.70	0	12,15,17	1.70	2 (16%)
2	BGC	C	5	2	11,11,12	0.56	0	15,15,17	1.92	4 (26%)
2	FUC	D	1	2	10,10,11	0.44	0	14,14,16	1.03	1 (7%)
2	GAL	D	2	2	12,12,12	1.27	2 (16%)	17,17,17	2.44	4 (23%)
2	NAG	D	3	2	14,14,15	2.00	3 (21%)	12,19,21	5.22	3 (25%)
2	GAL	D	4	2	11,11,12	0.98	0	12,15,17	2.54	4 (33%)
2	BGC	D	5	2	11,11,12	0.84	0	15,15,17	2.22	4 (26%)
2	NAG	D	532	2	14,14,15	0.64	0	12,19,21	1.24	2 (16%)
2	GAL	D	533	2	12,12,12	0.48	0	17,17,17	0.76	1 (5%)
2	FUC	D	534	2	10,10,11	0.43	0	14,14,16	1.01	1 (7%)
2	GAL	D	535	2	11,11,12	0.57	0	12,15,17	1.14	2 (16%)
2	BGC	D	536	2	11,11,12	0.56	0	15,15,17	0.98	2 (13%)
2	FUC	E	1	2	10,10,11	0.43	0	14,14,16	1.01	1 (7%)
2	GAL	E	2	2	12,12,12	0.48	0	17,17,17	0.75	1 (5%)
4	NAG	E	3	3,4	14,14,15	1.03	0	12,19,21	2.08	5 (41%)
4	GAL	E	4	4	11,11,12	0.67	0	12,15,17	2.61	2 (16%)
4	BGC	E	5	4	11,11,12	0.74	0	15,15,17	1.98	4 (26%)
2	NAG	E	532	2	14,14,15	0.64	0	12,19,21	1.22	2 (16%)
2	GAL	E	533	2	11,11,12	0.58	0	12,15,17	1.14	2 (16%)
2	BGC	E	534	2	11,11,12	0.56	0	15,15,17	0.99	2 (13%)
2	FUC	G	1	2	10,10,11	0.44	0	14,14,16	1.01	1 (7%)
2	GAL	G	2	2	12,12,12	0.49	0	17,17,17	0.76	1 (5%)
2	NAG	G	3	2	14,14,15	0.63	0	12,19,21	1.23	2 (16%)
2	GAL	G	4	2	11,11,12	0.58	0	12,15,17	1.15	2 (16%)
2	BGC	G	5	2	11,11,12	0.57	0	15,15,17	0.98	2 (13%)
2	NAG	G	532	2	14,14,15	0.64	0	12,19,21	1.35	3 (25%)
2	GAL	G	533	2	12,12,12	0.48	0	17,17,17	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FUC	G	534	2	10,10,11	0.43	0	14,14,16	1.00	1 (7%)
2	GAL	G	535	2	11,11,12	0.59	0	12,15,17	1.14	2 (16%)
2	BGC	G	536	2	11,11,12	0.56	0	15,15,17	0.98	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	A	1	2	-	0/0/17/20	0/1/1/1
2	GAL	A	2	2	-	0/2/22/22	0/1/1/1
2	NAG	A	3	2	-	0/6/22/26	0/1/1/1
2	GAL	A	4	2	-	0/2/18/22	0/1/1/1
2	BGC	A	5	2	-	0/2/18/22	0/1/1/1
3	FUC	B	1	3	-	0/0/17/20	0/1/1/1
3	GAL	B	2	3,4	-	0/2/22/22	0/1/1/1
2	FUC	C	1	2	-	0/0/17/20	0/1/1/1
2	GAL	C	2	2	-	0/2/22/22	0/1/1/1
2	NAG	C	3	2	-	0/6/22/26	0/1/1/1
2	GAL	C	4	2	-	0/2/18/22	0/1/1/1
2	BGC	C	5	2	-	0/2/18/22	0/1/1/1
2	FUC	D	1	2	-	0/0/17/20	0/1/1/1
2	GAL	D	2	2	-	0/2/22/22	0/1/1/1
2	NAG	D	3	2	-	0/6/22/26	0/1/1/1
2	GAL	D	4	2	-	0/2/18/22	0/1/1/1
2	BGC	D	5	2	-	0/2/18/22	0/1/1/1
2	NAG	D	532	2	-	0/6/22/26	0/1/1/1
2	GAL	D	533	2	-	0/2/22/22	0/1/1/1
2	FUC	D	534	2	-	0/0/17/20	0/1/1/1
2	GAL	D	535	2	-	0/2/18/22	0/1/1/1
2	BGC	D	536	2	-	0/2/18/22	0/1/1/1
2	FUC	E	1	2	-	0/0/17/20	0/1/1/1
2	GAL	E	2	2	-	0/2/22/22	0/1/1/1
4	NAG	E	3	3,4	-	0/6/22/26	0/1/1/1
4	GAL	E	4	4	-	0/2/18/22	0/1/1/1
4	BGC	E	5	4	-	0/2/18/22	0/1/1/1
2	NAG	E	532	2	-	0/6/22/26	0/1/1/1
2	GAL	E	533	2	-	0/2/18/22	0/1/1/1
2	BGC	E	534	2	-	0/2/18/22	0/1/1/1
2	FUC	G	1	2	-	0/0/17/20	0/1/1/1
2	GAL	G	2	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	3	2	-	0/6/22/26	0/1/1/1
2	GAL	G	4	2	-	0/2/18/22	0/1/1/1
2	BGC	G	5	2	-	0/2/18/22	0/1/1/1
2	NAG	G	532	2	-	0/6/22/26	0/1/1/1
2	GAL	G	533	2	-	0/2/22/22	0/1/1/1
2	FUC	G	534	2	-	0/0/17/20	0/1/1/1
2	GAL	G	535	2	-	0/2/18/22	0/1/1/1
2	BGC	G	536	2	-	0/2/18/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	NAG	O1-C1	-4.28	1.24	1.39
2	A	3	NAG	O1-C1	-4.27	1.24	1.39
2	D	2	GAL	O5-C5	-2.93	1.37	1.44
2	A	2	GAL	O5-C5	-2.92	1.37	1.44
2	D	2	GAL	O5-C1	-2.58	1.38	1.43
2	A	2	GAL	O5-C1	-2.57	1.38	1.43
3	B	2	GAL	O5-C5	-2.53	1.38	1.44
2	C	1	FUC	C2-C3	-2.07	1.49	1.52
2	D	3	NAG	C3-C2	2.64	1.57	1.53
2	A	3	NAG	C3-C2	2.65	1.57	1.53
2	A	3	NAG	C1-C2	4.53	1.58	1.53
2	D	3	NAG	C1-C2	4.60	1.58	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	NAG	C6-C5-C4	-17.48	91.00	113.29
2	A	3	NAG	C6-C5-C4	-17.45	91.04	113.29
2	C	3	NAG	C6-C5-C4	-14.40	94.92	113.29
2	C	1	FUC	C6-C5-C4	-8.45	96.44	113.08
4	E	4	GAL	O5-C1-C2	-7.00	98.84	109.81
2	D	2	GAL	C1-O5-C5	-5.87	102.62	113.47
2	A	2	GAL	C1-O5-C5	-5.86	102.63	113.47
2	A	5	BGC	C4-C5-C6	-5.75	101.77	112.38
2	D	5	BGC	C4-C5-C6	-5.74	101.80	112.38
2	A	4	GAL	C6-C5-C4	-5.53	106.23	113.29
2	D	4	GAL	C6-C5-C4	-5.53	106.24	113.29
4	E	4	GAL	C6-C5-C4	-5.26	106.59	113.29
2	C	5	BGC	C3-C4-C5	-4.80	101.67	111.40
2	C	2	GAL	O5-C1-C2	-4.71	102.29	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	GAL	O5-C5-C4	-4.70	100.87	109.68
2	D	2	GAL	O5-C5-C4	-4.69	100.89	109.68
2	C	2	GAL	C6-C5-C4	-4.46	102.02	113.02
2	A	5	BGC	C3-C4-C5	-4.22	102.85	111.40
2	D	5	BGC	C3-C4-C5	-4.21	102.86	111.40
4	E	5	BGC	O5-C1-C2	-4.20	103.10	109.80
2	C	4	GAL	C1-O5-C5	-4.03	106.02	113.47
4	E	3	NAG	C6-C5-C4	-3.84	108.39	113.29
3	B	2	GAL	C1-O5-C5	-3.76	106.52	113.47
2	A	4	GAL	C1-O5-C5	-3.46	107.06	113.47
2	D	4	GAL	C1-O5-C5	-3.46	107.07	113.47
4	E	5	BGC	C1-C2-C3	-3.04	105.91	110.43
2	G	4	GAL	C6-C5-C4	-2.98	109.48	113.29
2	D	535	GAL	C6-C5-C4	-2.97	109.51	113.29
2	D	532	NAG	C6-C5-C4	-2.96	109.51	113.29
2	G	532	NAG	C6-C5-C4	-2.96	109.51	113.29
2	G	535	GAL	C6-C5-C4	-2.96	109.51	113.29
2	G	3	NAG	C6-C5-C4	-2.96	109.52	113.29
2	E	533	GAL	C6-C5-C4	-2.95	109.53	113.29
2	E	532	NAG	C6-C5-C4	-2.94	109.54	113.29
2	C	5	BGC	O5-C5-C4	-2.89	104.59	109.97
4	E	3	NAG	O4-C4-C3	-2.65	103.56	110.06
2	C	2	GAL	O2-C2-C3	-2.63	104.42	110.34
4	E	3	NAG	C1-O5-C5	-2.61	108.65	113.47
2	C	1	FUC	C1-C2-C3	-2.57	106.50	109.54
3	B	2	GAL	O5-C5-C4	-2.47	105.05	109.68
2	A	4	GAL	O5-C1-C2	-2.39	106.07	109.81
2	D	4	GAL	O5-C1-C2	-2.38	106.07	109.81
2	C	3	NAG	C1-O5-C5	-2.37	109.09	113.47
4	E	3	NAG	O6-C6-C5	-2.36	103.53	111.33
2	A	3	NAG	C3-C2-N2	-2.31	106.56	110.59
2	D	3	NAG	C3-C2-N2	-2.30	106.58	110.59
4	E	5	BGC	C4-C3-C2	-2.23	107.52	110.56
3	B	2	GAL	O3-C3-C4	-2.19	105.40	110.34
2	G	2	GAL	C1-O5-C5	-2.17	109.45	113.47
2	D	536	BGC	C1-O5-C5	-2.17	109.47	113.47
2	G	5	BGC	C1-O5-C5	-2.17	109.47	113.47
2	G	535	GAL	C1-O5-C5	-2.16	109.47	113.47
2	D	532	NAG	C1-O5-C5	-2.16	109.47	113.47
2	G	536	BGC	C1-O5-C5	-2.16	109.49	113.47
2	D	5	BGC	C4-C3-C2	-2.16	107.62	110.56
2	E	532	NAG	C1-O5-C5	-2.15	109.49	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	4	GAL	C1-O5-C5	-2.15	109.50	113.47
2	D	535	GAL	C1-O5-C5	-2.15	109.50	113.47
2	C	5	BGC	O1-C1-C2	-2.15	103.46	109.21
2	A	5	BGC	C4-C3-C2	-2.14	107.64	110.56
2	G	3	NAG	C1-O5-C5	-2.14	109.51	113.47
2	G	533	GAL	C1-O5-C5	-2.14	109.52	113.47
2	G	532	NAG	C1-O5-C5	-2.14	109.52	113.47
2	D	533	GAL	C1-O5-C5	-2.14	109.52	113.47
2	E	2	GAL	C1-O5-C5	-2.13	109.52	113.47
2	E	533	GAL	C1-O5-C5	-2.13	109.52	113.47
2	E	534	BGC	C1-O5-C5	-2.13	109.54	113.47
3	B	2	GAL	O4-C4-C3	-2.08	105.65	110.34
2	G	532	NAG	O6-C6-C5	-2.06	104.54	111.33
2	G	1	FUC	O5-C5-C6	2.02	109.47	106.13
2	D	1	FUC	O5-C5-C6	2.03	109.48	106.13
3	B	1	FUC	O5-C5-C6	2.04	109.50	106.13
2	E	1	FUC	O5-C5-C6	2.04	109.50	106.13
2	A	1	FUC	O5-C5-C6	2.04	109.50	106.13
2	D	534	FUC	O5-C5-C6	2.05	109.51	106.13
2	G	534	FUC	O5-C5-C6	2.05	109.52	106.13
2	C	2	GAL	O5-C5-C4	2.14	113.69	109.68
2	A	2	GAL	C6-C5-C4	2.23	118.52	113.02
2	D	2	GAL	C6-C5-C4	2.24	118.54	113.02
2	G	5	BGC	O5-C5-C6	2.30	109.44	106.62
2	D	536	BGC	O5-C5-C6	2.32	109.46	106.62
2	G	536	BGC	O5-C5-C6	2.33	109.47	106.62
2	A	3	NAG	O1-C1-O5	2.33	116.62	110.25
2	D	3	NAG	O1-C1-O5	2.34	116.64	110.25
2	E	534	BGC	O5-C5-C6	2.36	109.51	106.62
2	C	1	FUC	O5-C5-C4	2.48	113.82	109.53
2	C	5	BGC	O5-C5-C6	2.57	109.76	106.62
4	E	3	NAG	O5-C5-C6	2.75	113.31	106.36
2	A	5	BGC	O5-C5-C6	3.10	110.41	106.62
2	D	5	BGC	O5-C5-C6	3.10	110.42	106.62
2	C	4	GAL	O5-C5-C6	3.40	114.94	106.36
4	E	5	BGC	O1-C1-C2	3.77	119.31	109.21
2	C	2	GAL	C1-C2-C3	4.19	116.67	110.43
3	B	2	GAL	C1-C2-C3	4.29	116.81	110.43
2	D	2	GAL	C1-C2-C3	4.52	117.15	110.43
2	A	2	GAL	C1-C2-C3	4.52	117.15	110.43
2	D	4	GAL	O5-C5-C6	4.87	118.67	106.36
2	A	4	GAL	O5-C5-C6	4.88	118.68	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	GAL	1	0
2	A	3	NAG	2	0
2	A	4	GAL	11	0
2	A	5	BGC	10	0
3	B	1	FUC	1	0
3	B	2	GAL	1	0
2	C	3	NAG	2	0
2	C	4	GAL	3	0
2	C	5	BGC	1	0
2	D	2	GAL	2	0
2	D	3	NAG	3	0
2	D	4	GAL	12	1
2	D	5	BGC	11	1
2	D	532	NAG	2	0
2	D	533	GAL	1	0
2	D	534	FUC	10	0
2	D	535	GAL	3	0
2	D	536	BGC	1	0
2	E	2	GAL	1	0
4	E	3	NAG	1	0
4	E	4	GAL	3	0
4	E	5	BGC	4	0
2	E	532	NAG	2	0
2	E	533	GAL	8	0
2	E	534	BGC	6	0
2	G	1	FUC	4	0
2	G	2	GAL	4	0
2	G	4	GAL	2	0
2	G	5	BGC	2	0
2	G	532	NAG	6	0
2	G	533	GAL	2	0
2	G	534	FUC	5	0
2	G	535	GAL	9	0
2	G	536	BGC	7	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	309/311 (99%)	-0.32	2 (0%)	90	87	29, 41, 66, 80	0
1	B	308/311 (99%)	-0.46	1 (0%)	94	92	32, 44, 67, 78	0
1	C	311/311 (100%)	-0.23	2 (0%)	90	87	30, 45, 68, 93	0
1	D	307/311 (98%)	-0.32	1 (0%)	94	92	29, 45, 77, 95	0
1	E	309/311 (99%)	-0.20	4 (1%)	79	72	32, 47, 76, 89	0
1	F	308/311 (99%)	-0.12	3 (0%)	84	78	38, 57, 87, 103	0
1	G	308/311 (99%)	-0.23	1 (0%)	94	92	41, 57, 82, 118	0
1	H	292/311 (93%)	-0.20	4 (1%)	78	71	34, 59, 93, 117	0
1	I	285/311 (91%)	0.59	38 (13%)	4	2	52, 83, 121, 146	0
1	J	307/311 (98%)	-0.17	1 (0%)	94	92	38, 53, 84, 105	0
All	All	3044/3110 (97%)	-0.17	57 (1%)	70	61	29, 52, 89, 146	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	377	THR	5.7
1	I	369	THR	4.4
1	I	296	THR	4.2
1	I	295	GLY	3.7
1	H	299	TYR	3.5
1	H	370	ASP	3.5
1	I	508	VAL	3.5
1	C	412	ASP	3.4
1	E	412	ASP	3.2
1	I	292	HIS	3.1
1	I	300	THR	3.1
1	F	412	ASP	3.0
1	I	294	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	298	ASN	3.0
1	I	254	SER	3.0
1	I	334	LEU	3.0
1	I	310	ASN	3.0
1	I	337	THR	2.9
1	I	375	PHE	2.8
1	A	372	SER	2.8
1	I	511	PRO	2.8
1	I	376	GLU	2.8
1	C	340	ARG	2.7
1	I	297	GLN	2.7
1	I	345	ARG	2.7
1	I	304	ALA	2.6
1	F	484	ARG	2.6
1	E	524	PHE	2.6
1	I	293	ILE	2.6
1	I	314	THR	2.6
1	B	470	SER	2.6
1	I	481	ASP	2.6
1	I	299	TYR	2.5
1	I	483	GLY	2.5
1	I	440	GLY	2.5
1	I	307	ASN	2.5
1	H	348	LYS	2.4
1	E	414	HIS	2.4
1	I	222	SER	2.4
1	I	412	ASP	2.4
1	I	505	HIS	2.4
1	I	291	THR	2.4
1	F	413	SER	2.3
1	J	374	ASP	2.2
1	I	289	ASP	2.2
1	D	294	ALA	2.2
1	G	484	ARG	2.2
1	H	289	ASP	2.2
1	I	506	ASP	2.2
1	I	290	VAL	2.2
1	I	474	LEU	2.2
1	E	294	ALA	2.1
1	I	368	SER	2.1
1	I	312	ASP	2.1
1	I	386	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	336	GLN	2.0
1	A	294	ALA	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FUC	B	1	10/11	0.74	0.35	5.34	123,126,129,131	0
2	FUC	D	1	10/11	0.83	0.39	4.91	101,104,107,109	0
2	FUC	E	1	10/11	0.79	0.40	4.17	129,130,132,133	0
2	FUC	D	534	10/11	0.79	0.35	2.84	112,116,117,119	0
2	FUC	G	1	10/11	0.86	0.31	1.76	122,123,124,125	0
2	FUC	G	534	10/11	0.73	0.36	1.45	129,131,131,132	0
2	FUC	A	1	10/11	0.82	0.27	1.23	101,104,107,109	0
2	FUC	C	1	10/11	0.84	0.27	1.19	121,123,124,126	0
2	BGC	G	5	11/12	0.39	0.53	-	145,149,150,150	0
2	NAG	A	3	14/15	0.77	0.51	-	124,127,130,132	0
2	GAL	G	533	12/12	0.62	0.43	-	134,136,139,142	0
2	GAL	E	2	12/12	0.75	0.39	-	136,139,142,147	0
2	BGC	C	5	11/12	0.50	0.65	-	149,152,153,153	0
4	GAL	E	4	11/12	0.52	1.03	-	173,174,176,178	0
4	BGC	E	5	11/12	-0.17	1.77	-	179,181,181,182	0
2	NAG	D	3	14/15	0.78	0.53	-	124,127,130,132	0
2	BGC	E	534	11/12	0.54	0.88	-	162,163,164,164	0
2	BGC	D	536	11/12	0.69	0.59	-	145,146,147,147	0
2	GAL	A	4	11/12	0.71	0.77	-	133,135,137,139	0
2	GAL	E	533	11/12	0.78	0.78	-	160,162,163,163	0
2	GAL	D	4	11/12	0.45	0.48	-	133,135,137,139	0
2	GAL	D	535	11/12	0.79	0.59	-	144,146,147,147	0
4	NAG	E	3	14/15	0.32	0.80	-	161,162,166,169	0
2	BGC	G	536	11/12	0.42	0.70	-	156,158,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	C	3	14/15	0.75	0.53	-	138,140,144,147	0
2	NAG	G	532	14/15	0.54	0.77	-	146,147,149,151	0
3	GAL	B	2	12/12	0.50	0.54	-	137,144,148,155	0
2	GAL	D	2	12/12	0.66	0.44	-	115,121,122,125	0
2	GAL	D	533	12/12	0.72	0.45	-	124,129,131,134	0
2	GAL	C	2	12/12	0.82	0.41	-	130,134,135,137	0
2	GAL	G	2	12/12	0.77	0.44	-	129,132,135,138	0
2	NAG	D	532	14/15	0.75	0.60	-	132,135,139,142	0
2	GAL	A	2	12/12	0.69	0.40	-	115,121,122,125	0
2	GAL	C	4	11/12	0.29	0.75	-	149,151,153,153	0
2	BGC	A	5	11/12	0.80	0.78	-	140,141,141,141	0
2	GAL	G	535	11/12	0.59	0.54	-	151,153,154,155	0
2	GAL	G	4	11/12	0.57	0.50	-	145,147,148,148	0
2	BGC	D	5	11/12	0.37	0.56	-	140,141,141,141	0
2	NAG	G	3	14/15	0.77	0.58	-	139,142,143,145	0
2	NAG	E	532	14/15	0.71	0.80	-	152,153,156,158	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.