



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3OTK
Title : Structure and mechanisim of core 2 beta1,6-n-acetylglucosaminyltransferase:
a Metal-ion independent gt-a glycosyltransferase
Authors : Pak, J.E.; Rini, J.M.
Deposited on : 2010-09-13
Resolution : 2.30 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

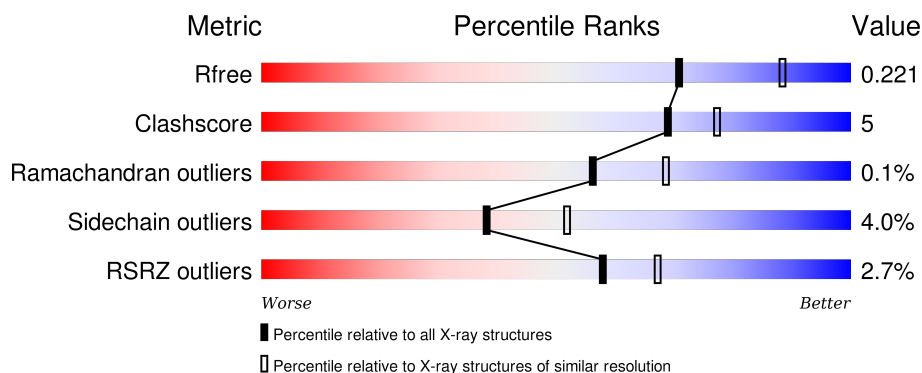
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	391	<div> <div>2%</div> <div>81% 14% 6%</div> </div>
1	B	391	<div> <div>3%</div> <div>80% 13% 7%</div> </div>
1	C	391	<div> <div>3%</div> <div>80% 11% 8%</div> </div>
1	D	391	<div> <div>%</div> <div>83% 9% 7%</div> </div>

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	HTO	A	584	-	-	-	X
2	HTO	A	585	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12658 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.

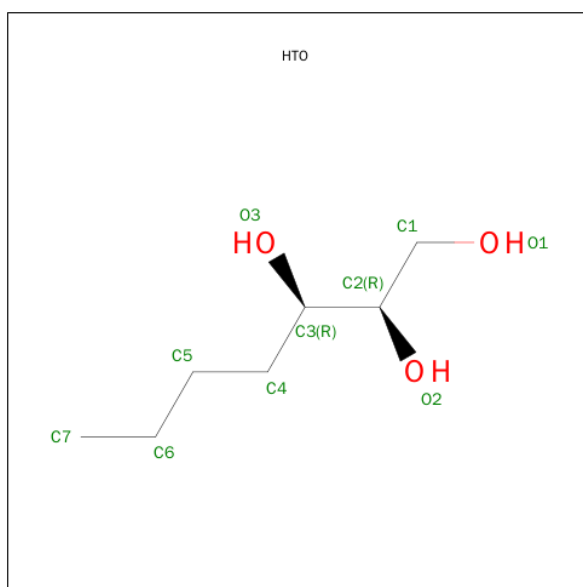
- Molecule 1 is a protein called Beta-1,3-galactosyl-O-glycosyl-glycoprotein beta-1,6-N-acetyl glucosaminyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	2	0
			3015	1936	513	545	21			
1	B	363	Total	C	N	O	S	0	1	0
			2956	1897	501	537	21			
1	C	360	Total	C	N	O	S	0	1	0
			2934	1881	498	535	20			
1	D	364	Total	C	N	O	S	0	2	0
			2966	1905	502	538	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	SER	CYS	ENGINEERED MUTATION	UNP Q09324
B	217	SER	CYS	ENGINEERED MUTATION	UNP Q09324
C	217	SER	CYS	ENGINEERED MUTATION	UNP Q09324
D	217	SER	CYS	ENGINEERED MUTATION	UNP Q09324

- Molecule 2 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).

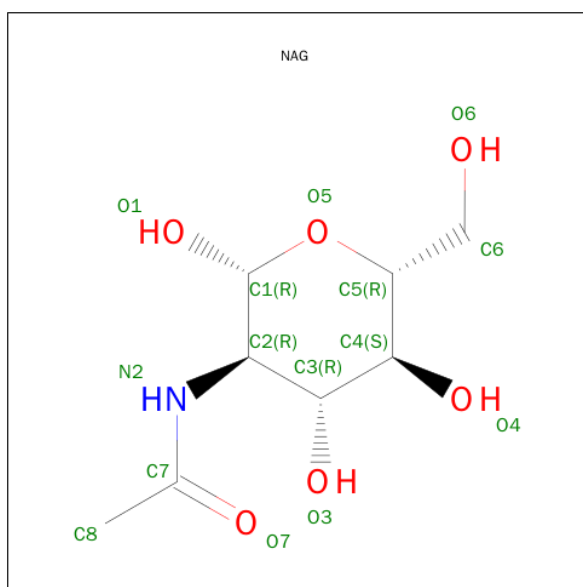


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	7	3		
2	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

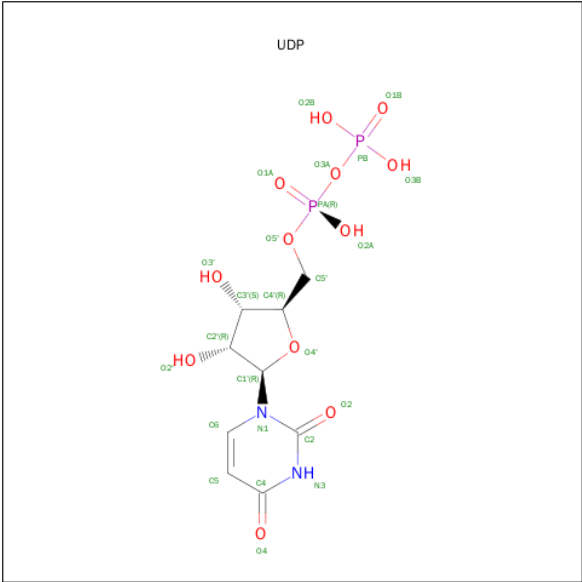


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		
5	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

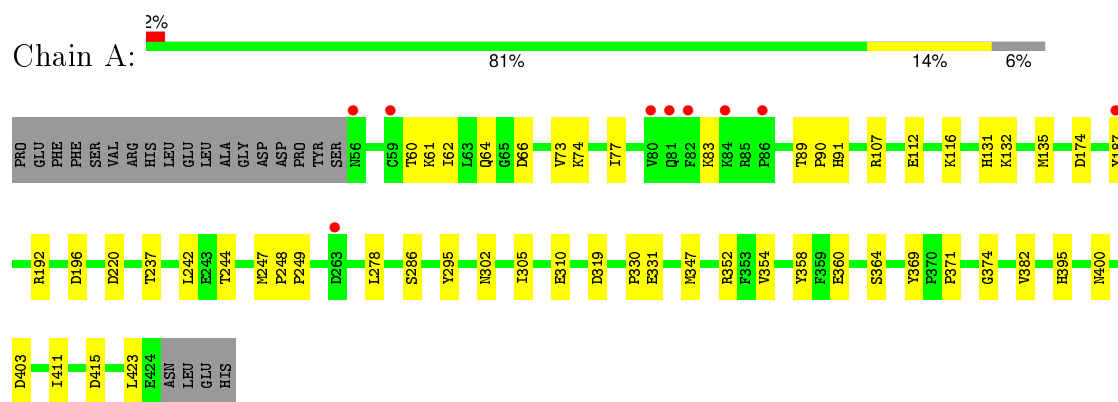
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	143	Total	O	0	0
			143	143		
7	B	122	Total	O	0	0
			122	122		
7	C	120	Total	O	0	0
			120	120		
7	D	148	Total	O	0	0
			148	148		

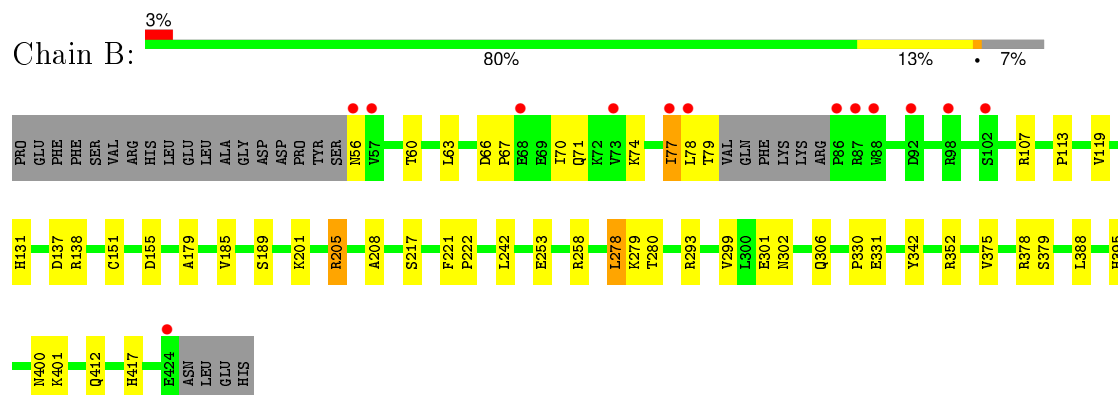
3 Residue-property plots [i](#)

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.

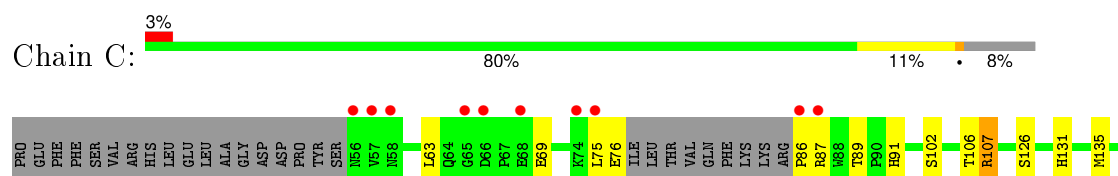
- Molecule 1: Beta-1,3-galactosyl-O-glycosyl-glycoprotein beta-1,6-N-acetylglucosaminyltransferase

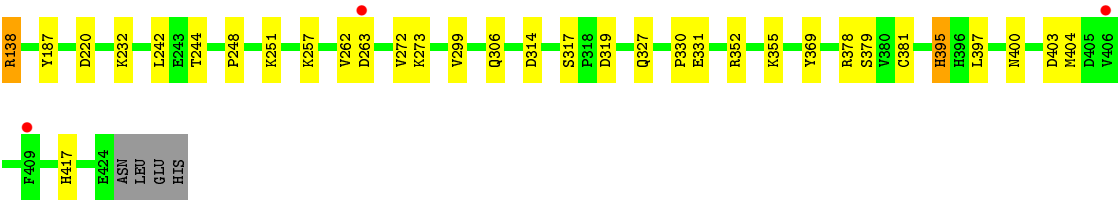


- Molecule 1: Beta-1,3-galactosyl-O-glycosyl-glycoprotein beta-1,6-N-acetylglucosaminyltransferase

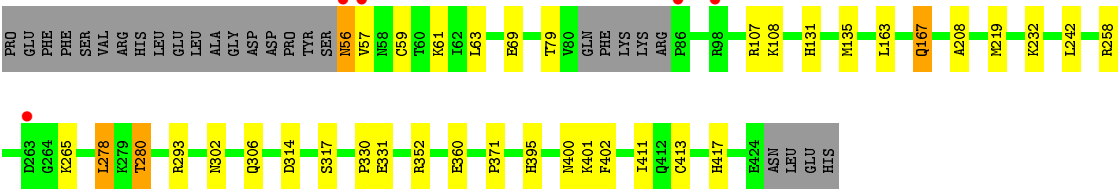
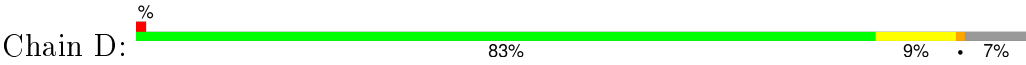


- Molecule 1: Beta-1,3-galactosyl-O-glycosyl-glycoprotein beta-1,6-N-acetylglucosaminyltransferase





● Molecule 1: Beta-1,3-galactosyl-O-glycosyl-glycoprotein beta-1,6-N-acetylglucosaminyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.87Å 101.02Å 136.61Å 90.00° 93.42° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.64 – 2.21	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.30) 93.5 (48.64-2.21)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.219 0.170 , 0.221	Depositor DCC
R_{free} test set	4291 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.1	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 93723 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12658	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HTO, NA, UDP, 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	0.46	0/3096	0.56	0/4197
1	B	0.44	0/3032	0.56	0/4110
1	C	0.44	0/3010	0.57	0/4080
1	D	0.45	0/3048	0.57	0/4132
All	All	0.45	0/12186	0.57	0/16519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3015	0	2984	32	0
1	B	2956	0	2916	28	0
1	C	2934	0	2881	32	0
1	D	2966	0	2934	20	0
2	A	20	0	32	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	38	0	34	0	0
5	C	38	0	34	0	0
6	A	25	0	11	2	0
6	B	25	0	11	1	0
6	C	25	0	11	2	0
6	D	25	0	11	0	0
7	A	143	0	0	0	0
7	B	122	0	0	1	0
7	C	120	0	0	1	0
7	D	148	0	0	1	0
All	All	12658	0	11911	110	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 5.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:HG22	1:A:91:HIS:H	1.22	1.04
1:A:89:THR:HG23	1:A:90:PRO:HD2	1.48	0.94
1:C:135:MET:HE2	1:C:404:MET:H	1.43	0.83
1:D:302:ASN:O	1:D:306:GLN:HG2	1.79	0.82
1:C:187:TYR:HE1	6:C:600:UDP:O3B	1.62	0.82
1:A:330:PRO:O	1:A:331:GLU:HB2	1.81	0.79
1:D:163:LEU:O	1:D:167:GLN:HG2	1.87	0.74
1:A:89:THR:HG22	1:A:91:HIS:N	2.00	0.74
1:B:258:ARG:HD3	7:B:439:HOH:O	1.88	0.72
1:B:278:LEU:HD13	1:B:280:THR:O	1.89	0.71
1:C:330:PRO:O	1:C:331:GLU:HB2	1.90	0.71
1:C:220:ASP:OD1	1:C:400:ASN:HB2	1.93	0.69
1:D:61:LYS:CB	1:D:69:GLU:HG3	2.24	0.68
1:B:66:ASP:O	1:B:70:ILE:HG12	1.96	0.65
1:B:138:ARG:HH22	1:B:412:GLN:HG2	1.62	0.65
1:C:63:LEU:HD11	1:C:417:HIS:HB2	1.80	0.64
1:A:89:THR:HG23	1:A:90:PRO:CD	2.25	0.63
1:D:61:LYS:HB2	1:D:69:GLU:HG3	1.82	0.61
1:C:248:PRO:HG2	1:C:251:LYS:HG3	1.83	0.60
1:D:56:ASN:HD22	1:D:57:VAL:N	2.00	0.60
1:C:89:THR:HG23	1:C:91:HIS:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ARG:HH22	1:C:404:MET:CB	2.14	0.60
1:B:201:LYS:O	1:B:205:ARG:HG2	2.02	0.60
1:D:258:ARG:HG3	1:D:314:ASP:OD2	2.03	0.59
1:A:132:LYS:HD3	1:A:135[A]:MET:CE	2.32	0.59
1:B:155:ASP:OD1	1:B:185:VAL:HB	2.03	0.59
1:B:330:PRO:O	1:B:331:GLU:HB2	2.01	0.58
1:A:60:THR:O	1:A:64:GLN:HG3	2.04	0.58
1:D:63:LEU:HD11	1:D:417:HIS:HB2	1.85	0.57
1:C:135:MET:HE2	1:C:404:MET:N	2.17	0.57
1:D:135[A]:MET:CE	1:D:219:MET:HG2	2.35	0.56
1:B:107:ARG:HD3	1:B:137:ASP:OD2	2.06	0.56
1:B:77:ILE:HG22	1:B:78:LEU:N	2.18	0.56
1:C:69:GLU:HA	1:C:69:GLU:OE2	2.04	0.56
1:B:217:SER:HB2	6:B:599:UDP:O3'	2.05	0.55
1:A:220:ASP:OD1	1:A:400:ASN:HB2	2.07	0.55
1:A:364:SER:O	1:B:279:LYS:HE2	2.07	0.54
1:C:135:MET:HE1	1:C:403:ASP:OD1	2.07	0.53
1:D:278:LEU:HD13	1:D:280:THR:O	2.08	0.53
1:B:63:LEU:HD11	1:B:417:HIS:HB2	1.90	0.53
1:C:262:VAL:O	1:C:263:ASP:HB2	2.09	0.53
1:B:71:GLN:HA	1:B:74:LYS:HB2	1.90	0.52
1:A:360:GLU:HB3	1:A:371:PRO:HA	1.92	0.52
1:A:347:MET:HE2	1:B:342:TYR:OH	2.09	0.52
1:D:330:PRO:O	1:D:331:GLU:HB2	2.09	0.51
1:B:302:ASN:O	1:B:306:GLN:HG2	2.10	0.50
1:C:89:THR:HG23	1:C:91:HIS:N	2.27	0.50
1:C:87:ARG:HH22	1:C:404:MET:HB3	1.76	0.50
1:D:258:ARG:HD3	7:D:451:HOH:O	2.12	0.49
1:A:374:GLY:HA3	1:A:382:VAL:O	2.12	0.49
1:A:116:LYS:HG3	2:A:584:HTO:H42	1.94	0.48
1:D:61:LYS:HB3	1:D:69:GLU:HG3	1.94	0.48
1:B:400:ASN:HA	1:B:401:LYS:HA	1.69	0.48
2:A:585:HTO:H3	6:A:598:UDP:O2B	2.14	0.48
1:B:208:ALA:HA	1:B:293:ARG:CZ	2.44	0.48
1:A:89:THR:CG2	1:A:90:PRO:HD2	2.33	0.48
1:C:86:PRO:O	1:C:87:ARG:HD2	2.14	0.47
1:C:327:GLN:HG3	1:C:327:GLN:O	2.14	0.47
1:C:107:ARG:NH1	7:C:508:HOH:O	2.37	0.47
1:D:400:ASN:HA	1:D:401:LYS:HA	1.68	0.47
1:B:378:ARG:O	1:B:379:SER:HB2	2.14	0.46
1:C:63:LEU:CD1	1:C:417:HIS:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:OE1	1:B:253:GLU:HA	2.17	0.45
1:C:232:LYS:HE3	1:C:232:LYS:HB3	1.82	0.45
1:A:73:VAL:O	1:A:77:ILE:HG12	2.17	0.45
1:A:83:LYS:HE2	1:A:83:LYS:HB3	1.86	0.44
1:C:187:TYR:CE1	6:C:600:UDP:O3B	2.55	0.44
1:A:347:MET:CE	1:B:342:TYR:OH	2.65	0.44
1:A:187:TYR:HE1	6:A:598:UDP:O3B	2.01	0.44
1:C:232:LYS:HD3	1:C:397:LEU:CD2	2.48	0.44
1:A:187:TYR:CE2	2:A:585:HTO:H73	2.52	0.43
1:D:59:CYS:HG	1:D:413:CYS:HG	1.60	0.43
1:A:62:ILE:HD11	1:A:73:VAL:HG21	2.00	0.43
1:B:258:ARG:HB2	1:B:258:ARG:HE	1.67	0.43
1:B:113:PRO:HB3	1:B:119:VAL:HG23	2.00	0.43
1:D:360:GLU:HB3	1:D:371:PRO:HA	2.01	0.43
1:C:102:SER:O	1:C:106:THR:HB	2.18	0.42
1:C:355:LYS:HB2	1:C:381:CYS:HB3	2.01	0.42
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.93	0.42
1:A:411:ILE:O	1:A:415:ASP:HB2	2.20	0.42
1:C:75:LEU:HB2	1:C:76:GLU:H	1.69	0.42
1:D:208:ALA:HA	1:D:293:ARG:CZ	2.49	0.42
1:A:74:LYS:NZ	1:A:74:LYS:HB3	2.34	0.42
1:D:232:LYS:HE3	1:D:232:LYS:HB3	1.85	0.42
1:A:192:ARG:NH1	1:A:196:ASP:OD2	2.47	0.42
1:A:89:THR:CG2	1:A:90:PRO:CD	2.94	0.42
1:C:273:LYS:NZ	1:C:314:ASP:OD1	2.43	0.42
1:A:89:THR:CG2	1:A:90:PRO:N	2.83	0.41
1:B:78:LEU:HA	1:B:78:LEU:HD12	1.95	0.41
1:C:107:ARG:HE	1:C:107:ARG:HA	1.85	0.41
1:A:302:ASN:OD1	1:A:305:ILE:HG12	2.20	0.41
1:C:138:ARG:HE	1:C:404:MET:CE	2.33	0.41
1:B:66:ASP:HA	1:B:67:PRO:HD3	1.92	0.41
1:B:221:PHE:CD2	1:B:222:PRO:HD2	2.56	0.41
1:D:107:ARG:O	1:D:108:LYS:HB2	2.21	0.41
1:B:151:CYS:SG	1:B:179:ALA:HB2	2.61	0.41
1:C:232:LYS:HE2	1:C:395:HIS:O	2.19	0.41
1:D:265:LYS:HE3	1:D:265:LYS:HB3	1.92	0.41
1:A:295:TYR:C	1:A:295:TYR:CD2	2.94	0.41
1:A:135[A]:MET:SD	1:A:403:ASP:HA	2.60	0.41
1:A:354:VAL:HG22	1:A:400:ASN:HB3	2.03	0.41
1:A:247:MET:HA	1:A:248:PRO:HD2	1.96	0.41
1:A:61:LYS:HD3	1:A:66:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PRO:O	1:B:331:GLU:CB	2.69	0.41
2:A:585:HTO:H52	2:A:585:HTO:O2	2.21	0.41
1:C:257:LYS:HE2	1:C:272:VAL:HG22	2.02	0.40
1:C:87:ARG:HH22	1:C:404:MET:HB2	1.87	0.40
1:D:402:PHE:CB	1:D:411:ILE:HD11	2.51	0.40
1:B:375:VAL:HG12	1:C:75:LEU:HD22	2.02	0.40
1:C:378:ARG:O	1:C:379:SER:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/391 (94%)	359 (97%)	9 (2%)	1 (0%)	46	57
1	B	360/391 (92%)	354 (98%)	6 (2%)	0	100	100
1	C	357/391 (91%)	344 (96%)	13 (4%)	0	100	100
1	D	362/391 (93%)	354 (98%)	8 (2%)	0	100	100
All	All	1448/1564 (93%)	1411 (97%)	36 (2%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LEU

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	333/351 (95%)	318 (96%)	15 (4%)	34	46
1	B	326/351 (93%)	312 (96%)	14 (4%)	35	47
1	C	323/351 (92%)	310 (96%)	13 (4%)	38	52
1	D	328/351 (93%)	318 (97%)	10 (3%)	48	65
All	All	1310/1404 (93%)	1258 (96%)	52 (4%)	38	52

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	112	GLU
1	A	131	HIS
1	A	174	ASP
1	A	237	THR
1	A	242	LEU
1	A	244	THR
1	A	278	LEU
1	A	286	SER
1	A	310	GLU
1	A	319	ASP
1	A	352	ARG
1	A	358	TYR
1	A	369	TYR
1	A	395	HIS
1	B	56	ASN
1	B	60	THR
1	B	77	ILE
1	B	79	THR
1	B	131	HIS
1	B	189	SER
1	B	205	ARG
1	B	242	LEU
1	B	278	LEU
1	B	299	VAL
1	B	301	GLU
1	B	352	ARG
1	B	388	LEU
1	B	395	HIS
1	C	107	ARG

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Mol	Chain	Res	Type
1	C	126	SER
1	C	131	HIS
1	C	138	ARG
1	C	242	LEU
1	C	244	THR
1	C	299	VAL
1	C	306	GLN
1	C	317	SER
1	C	319	ASP
1	C	352	ARG
1	C	369	TYR
1	C	395	HIS
1	D	56	ASN
1	D	79	THR
1	D	131	HIS
1	D	167	GLN
1	D	242	LEU
1	D	278	LEU
1	D	280	THR
1	D	317	SER
1	D	352	ARG
1	D	395	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	B	181	GLN
1	B	209	ASN
1	B	313	GLN
1	B	340	ASN
1	B	396	HIS
1	D	56	ASN
1	D	306	GLN
1	D	313	GLN
1	D	340	ASN
1	D	400	ASN

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 ⓘ

6 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	$\# Z > 2$
5	NAG	A	589	1,5	14,14,15	0.56	0	15,19,21	1.55	2 (13%)
5	NAG	A	590	5	14,14,15	0.53	0	15,19,21	0.74	0
5	FUC	A	591	5	10,10,11	0.60	0	14,14,16	0.99	1 (7%)
5	NAG	C	594	1,5	14,14,15	0.58	0	15,19,21	1.30	1 (6%)
5	NAG	C	595	5	14,14,15	0.50	0	15,19,21	0.80	0
5	FUC	C	596	5	10,10,11	0.66	0	14,14,16	1.15	2 (14%)

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
5	NAG	A	589	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	590	5	-	0/6/23/26	0/1/1/1
5	FUC	A	591	5	-	0/0/17/20	0/1/1/1
5	NAG	C	594	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	595	5	-	0/6/23/26	0/1/1/1
5	FUC	C	596	5	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	596	FUC	O5-C1-C2	-2.41	106.95	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	589	NAG	C3-C2-N2	-2.17	105.37	110.56
5	C	596	FUC	O5-C5-C6	2.46	110.19	106.13
5	A	591	FUC	O5-C5-C6	2.96	111.02	106.13
5	C	594	NAG	C1-O5-C5	4.02	117.35	112.25
5	A	589	NAG	C1-O5-C5	4.81	118.36	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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	HTO	A	584	-	9,9,9	0.43	0	8,10,10	0.61	0
2	HTO	A	585	-	9,9,9	0.35	0	8,10,10	0.81	0
4	NAG	A	588	1	14,14,15	0.48	0	15,19,21	0.95	1 (6%)
6	UDP	A	598	-	18,26,26	1.13	1 (5%)	26,40,40	1.83	3 (11%)
4	NAG	B	592	1	14,14,15	0.44	0	15,19,21	0.72	0
6	UDP	B	599	-	18,26,26	1.19	1 (5%)	26,40,40	1.53	3 (11%)
4	NAG	C	593	1	14,14,15	0.44	0	15,19,21	1.08	1 (6%)
6	UDP	C	600	-	18,26,26	1.15	1 (5%)	26,40,40	1.45	2 (7%)
4	NAG	D	597	1	14,14,15	0.50	0	15,19,21	0.80	0
6	UDP	D	601	-	18,26,26	1.23	1 (5%)	26,40,40	1.55	2 (7%)

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	HTO	A	584	-	-	0/10/10/10	0/0/0/0
2	HTO	A	585	-	-	0/10/10/10	0/0/0/0
4	NAG	A	588	1	-	0/6/23/26	0/1/1/1
6	UDP	A	598	-	-	0/12/32/32	0/2/2/2
4	NAG	B	592	1	-	0/6/23/26	0/1/1/1
6	UDP	B	599	-	-	0/12/32/32	0/2/2/2
4	NAG	C	593	1	-	0/6/23/26	0/1/1/1
6	UDP	C	600	-	-	0/12/32/32	0/2/2/2
4	NAG	D	597	1	-	0/6/23/26	0/1/1/1
6	UDP	D	601	-	-	0/12/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	598	UDP	C4-N3	2.71	1.38	1.33
6	C	600	UDP	C4-N3	2.77	1.38	1.33
6	B	599	UDP	C4-N3	2.82	1.38	1.33
6	D	601	UDP	C4-N3	3.11	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	598	UDP	PA-O3A-PB	-4.58	117.32	132.67
6	D	601	UDP	PA-O3A-PB	-3.43	121.16	132.67
6	B	599	UDP	PA-O3A-PB	-2.73	123.52	132.67
6	C	600	UDP	PA-O3A-PB	-2.28	125.03	132.67
4	A	588	NAG	O5-C5-C6	2.28	112.29	107.35
6	A	598	UDP	O4'-C1'-N1	2.29	112.91	108.08
6	B	599	UDP	O4'-C1'-N1	2.32	112.98	108.08
4	C	593	NAG	C1-O5-C5	3.14	116.24	112.25
6	B	599	UDP	C4-N3-C2	5.89	119.97	114.14
6	C	600	UDP	C4-N3-C2	5.89	119.98	114.14
6	D	601	UDP	C4-N3-C2	5.95	120.04	114.14
6	A	598	UDP	C4-N3-C2	6.70	120.77	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	584	HTO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	585	HTO	3	0
6	A	598	UDP	2	0
6	B	599	UDP	1	0
6	C	600	UDP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	369/391 (94%)	-0.36	9 (2%) 62 71	23, 38, 66, 96	0
1	B	363/391 (92%)	-0.10	13 (3%) 46 55	24, 42, 76, 103	0
1	C	360/391 (92%)	-0.22	13 (3%) 46 55	22, 39, 73, 95	0
1	D	364/391 (93%)	-0.23	5 (1%) 78 83	22, 39, 63, 88	0
All	All	1456/1564 (93%)	-0.23	40 (2%) 58 67	22, 39, 71, 103	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	PRO	6.1
1	C	87	ARG	5.7
1	C	56	ASN	5.1
1	C	86	PRO	4.2
1	B	77	ILE	4.0
1	B	88	TRP	3.5
1	A	80	VAL	3.3
1	B	57	VAL	3.3
1	C	75	LEU	3.2
1	C	68	GLU	3.2
1	A	81	GLN	3.1
1	D	57	VAL	3.0
1	D	86	PRO	2.9
1	B	102	SER	2.9
1	B	56	ASN	2.9
1	A	82	PHE	2.8
1	D	263	ASP	2.8
1	C	406	VAL	2.7
1	C	409	PHE	2.7
1	D	56	ASN	2.6
1	A	84	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	57	VAL	2.6
1	B	87	ARG	2.5
1	B	92	ASP	2.5
1	A	56	ASN	2.4
1	A	59	CYS	2.4
1	A	263	ASP	2.4
1	B	98	ARG	2.4
1	C	66	ASP	2.3
1	A	86	PRO	2.3
1	C	65	GLY	2.3
1	B	68	GLU	2.3
1	C	74	LYS	2.1
1	A	187	TYR	2.1
1	B	73	VAL	2.1
1	B	424	GLU	2.1
1	B	78	LEU	2.1
1	D	98	ARG	2.1
1	C	263	ASP	2.1
1	C	58	ASN	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(Å ²)	Q<0.9
5	NAG	C	594	14/15	0.94	0.13	0.36	37,52,65,70	0
5	NAG	A	589	14/15	0.93	0.10	-0.67	38,57,67,67	0
5	NAG	C	595	14/15	0.89	0.35	-	51,91,120,122	0
5	NAG	A	590	14/15	0.96	0.18	-	48,80,98,100	0
5	FUC	A	591	10/11	0.94	0.21	-	45,68,78,86	0
5	FUC	C	596	10/11	0.93	0.26	-	60,66,79,86	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	HTO	A	584	10/10	0.69	0.26	8.41	47,84,110,113	0
2	HTO	A	585	10/10	0.78	0.19	2.09	42,64,75,77	0
6	UDP	B	599	25/25	0.91	0.13	0.34	33,63,149,157	0
6	UDP	A	598	25/25	0.97	0.11	0.02	27,40,65,90	0
6	UDP	C	600	25/25	0.96	0.10	-0.40	36,53,73,90	0
6	UDP	D	601	25/25	0.92	0.12	-0.48	33,59,142,152	0
3	NA	C	587	1/1	0.96	0.08	-1.24	38,38,38,38	0
3	NA	A	586	1/1	0.82	0.07	-1.99	43,43,43,43	0
4	NAG	D	597	14/15	0.73	0.22	-	82,105,118,118	0
4	NAG	B	592	14/15	0.74	0.30	-	94,112,124,125	0
4	NAG	A	588	14/15	0.89	0.20	-	73,93,107,125	0
4	NAG	C	593	14/15	0.65	0.23	-	75,105,122,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.