



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:02 PM GMT

PDB ID : 4GYW
Title : Crystal structure of human O-GlcNAc Transferase in complex with UDP and a glycopeptide
Authors : Lazarus, M.B.; Jiang, J.; Gloster, T.M.; Zandberg, W.F.; Vocadlo, D.J.; Walker, S.
Deposited on : 2012-09-05
Resolution : 1.70 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

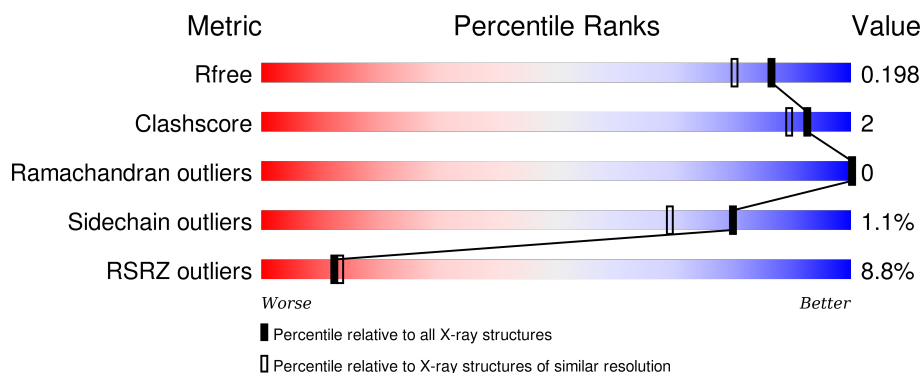
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	723	<div> <div>8%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	C	723	<div> <div>8%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
2	B	14	<div> <div>14%</div> <div>79%</div> <div>21%</div> </div>
2	D	14	<div> <div>14%</div> <div>71%</div> <div>29%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12156 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	8	0
			5536	3514	966	1019	37			
1	C	674	Total	C	N	O	S	0	7	0
			5367	3417	934	978	38			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	EXPRESSION TAG	UNP O15294
A	310	PRO	-	EXPRESSION TAG	UNP O15294
A	311	GLY	-	EXPRESSION TAG	UNP O15294
A	312	SER	-	EXPRESSION TAG	UNP O15294
C	309	GLY	-	EXPRESSION TAG	UNP O15294
C	310	PRO	-	EXPRESSION TAG	UNP O15294
C	311	GLY	-	EXPRESSION TAG	UNP O15294
C	312	SER	-	EXPRESSION TAG	UNP O15294

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			
2	D	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	TYR	-	EXPRESSION TAG	UNP P68400
D	13	TYR	-	EXPRESSION TAG	UNP P68400

-
- The chemical structure of UDP (Uridine Diphosphate) is shown, consisting of a uracil base, a ribose sugar, and a diphosphate group. The uracil base is a six-membered ring with nitrogen atoms at positions 1 and 3, and carbonyl groups at positions 2 and 4. The ribose sugar is a five-membered ring with hydroxyl groups at positions 2' and 3'. The diphosphate group is attached to the 5' carbon of the ribose sugar. The structure is labeled with atom names and numbers, including N1, N3, C2, C4, C5, C6, C1', C2', C3', C4', C5', O1A, O1B, O2A, O2B, O3A, O3B, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O7

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

-

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

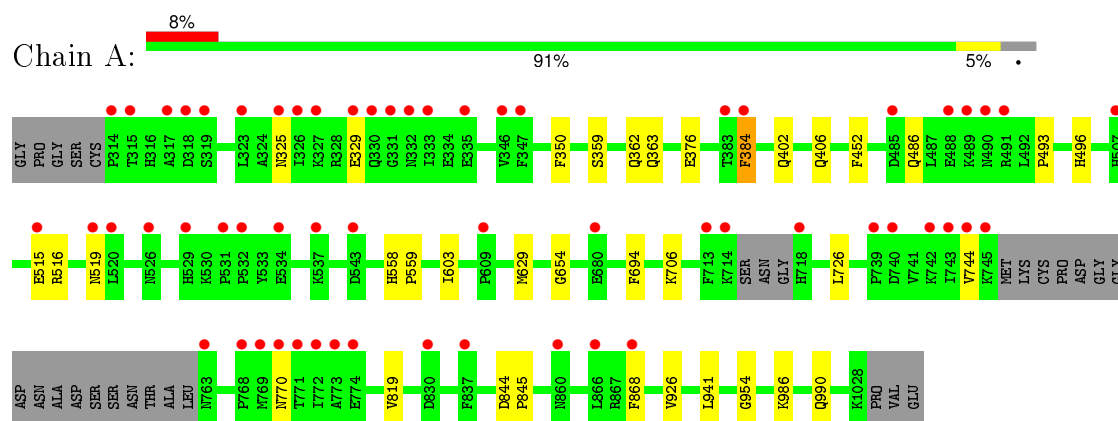
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	487	Total	O	0	0
			487	487		
6	B	19	Total	O	0	0
			19	19		
6	C	450	Total	O	0	0
			450	450		
6	D	14	Total	O	0	0
			14	14		

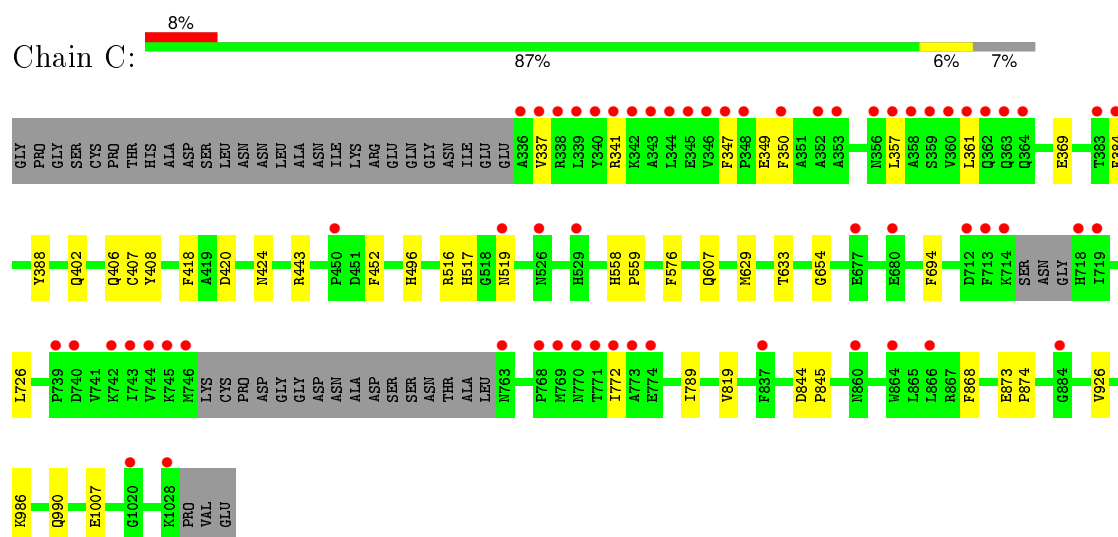
3 Residue-property plots [i](#)

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.

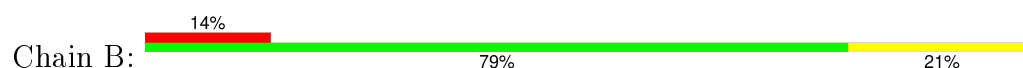
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



- Molecule 2: Casein kinase II subunit alpha





- Molecule 2: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.00 Å 137.77 Å 153.57 Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	43.90 – 1.70 43.90 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.2 (43.90-1.70) 94.2 (43.90-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.70 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.187 , 0.205 0.179 , 0.198	Depositor DCC
R_{free} test set	10313 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 206949 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: UDP, NAG, SO4

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	0.30	0/5688	0.48	0/7713
1	C	0.30	0/5515	0.48	0/7478
2	B	0.32	0/97	0.45	0/131
2	D	0.29	0/97	0.42	0/131
All	All	0.30	0/11397	0.48	0/15453

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	5536	0	5520	20	0
1	C	5367	0	5363	22	0
2	B	95	0	87	2	0
2	D	95	0	87	3	0
3	A	25	0	11	0	0
3	C	25	0	11	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	0	0
5	D	14	0	13	0	0
6	A	487	0	0	5	0
6	B	19	0	0	0	0
6	C	450	0	0	3	0
6	D	14	0	0	0	0
All	All	12156	0	11105	44	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 2.

All (44) 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:D:13:TYR:N	2:D:18:THR:HG1	1.92	0.68
1:A:726:LEU:CD2	1:A:819:VAL:HG22	2.26	0.66
2:B:13:TYR:N	2:B:18:THR:HG1	1.97	0.62
1:A:706:LYS:HE3	6:A:1654:HOH:O	2.04	0.58
1:A:986:LYS:HG3	1:A:990[B]:GLN:OE1	2.04	0.56
1:C:443:ARG:NH2	6:C:1621:HOH:O	2.36	0.56
1:C:726[A]:LEU:CD2	1:C:819:VAL:HG22	2.37	0.55
1:C:607:GLN:NE2	6:C:1582:HOH:O	2.39	0.54
1:C:986:LYS:HG3	1:C:990[B]:GLN:OE1	2.09	0.53
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.46	0.50
1:A:376:GLU:HG2	6:A:1424:HOH:O	2.12	0.50
1:A:402:GLN:O	1:A:406:GLN:HG2	2.12	0.49
1:C:772:ILE:HG23	1:C:789:ILE:HD13	1.94	0.48
1:A:325:ASN:O	1:A:329:GLU:HG2	2.14	0.47
1:C:337:VAL:O	1:C:341:ARG:HG3	2.14	0.47
1:A:770:ASN:ND2	6:A:1682:HOH:O	2.47	0.47
1:A:954:GLY:O	1:A:986:LYS:HE2	2.16	0.46
1:C:516:ARG:NH2	1:C:519:ASN:OD1	2.48	0.46
1:A:496:HIS:CE1	2:B:23:ALA:HB1	2.51	0.46
1:A:362:GLN:HG2	6:A:1639:HOH:O	2.15	0.46
1:C:402:GLN:O	1:C:406:GLN:HG2	2.17	0.45
1:A:359:SER:O	1:A:363:GLN:HG3	2.17	0.44
1:C:517:HIS:NE2	6:C:1569:HOH:O	2.31	0.44
1:C:347:PHE:CE1	1:C:349:GLU:HB2	2.53	0.44
1:A:516:ARG:NH2	6:A:1680:HOH:O	2.51	0.43
1:C:496:HIS:CE1	2:D:23:ALA:HB1	2.53	0.43
1:C:558:HIS:CG	1:C:559:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.55	0.42
1:C:629:MET:O	1:C:654:GLY:HA3	2.20	0.42
1:A:515[A]:GLU:OE2	1:A:519:ASN:ND2	2.51	0.42
1:A:486:GLN:OE1	1:A:493:PRO:HA	2.19	0.42
1:C:361:LEU:HD13	1:C:369:GLU:HB3	2.02	0.41
1:C:576:PHE:CZ	1:C:1007:GLU:HB3	2.55	0.41
1:C:844:ASP:HB2	1:C:845:PRO:HD2	2.01	0.41
1:A:844:ASP:HB2	1:A:845:PRO:HD2	2.01	0.41
1:A:603:ILE:N	1:A:603:ILE:HD12	2.35	0.41
1:C:873:GLU:N	1:C:874:PRO:HD2	2.36	0.41
1:C:418:PHE:CE1	1:C:420:ASP:HB2	2.55	0.41
1:A:941:LEU:HD23	1:A:941:LEU:C	2.41	0.41
1:A:629:MET:O	1:A:654:GLY:HA3	2.21	0.40
1:C:388:TYR:O	1:C:407:CYS:HB3	2.21	0.40
1:C:633:THR:O	2:D:24:ASN:HB3	2.21	0.40
1:C:357:LEU:O	1:C:361:LEU:HG	2.21	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	698/723 (96%)	686 (98%)	12 (2%)	0	100	100
1	C	675/723 (93%)	663 (98%)	12 (2%)	0	100	100
2	B	12/14 (86%)	12 (100%)	0	0	100	100
2	D	12/14 (86%)	12 (100%)	0	0	100	100
All	All	1397/1474 (95%)	1373 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	606/618 (98%)	599 (99%)	7 (1%)	78	65
1	C	586/618 (95%)	580 (99%)	6 (1%)	82	72
2	B	11/11 (100%)	11 (100%)	0	100	100
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	1214/1258 (96%)	1201 (99%)	13 (1%)	80	69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	PHE
1	A	384	PHE
1	A	452	PHE
1	A	694	PHE
1	A	744	VAL
1	A	868	PHE
1	A	926	VAL
1	C	350	PHE
1	C	384	PHE
1	C	452	PHE
1	C	694	PHE
1	C	868	PHE
1	C	926	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	GLN
1	A	763	ASN
1	C	607	GLN
1	C	784	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 ligands 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$
3	UDP	A	1101	-	18,26,26	1.20	1 (5%)	26,40,40	1.57	1 (3%)
4	SO4	A	1102	-	4,4,4	0.24	0	6,6,6	0.07	0
5	NAG	B	101	2	14,14,15	0.50	0	15,19,21	0.82	1 (6%)
4	SO4	B	102	-	4,4,4	0.20	0	6,6,6	0.07	0
3	UDP	C	1101	-	18,26,26	1.14	2 (11%)	26,40,40	1.45	1 (3%)
5	NAG	D	101	2	14,14,15	0.40	0	15,19,21	0.87	0
4	SO4	D	102	-	4,4,4	0.24	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	A	1101	-	-	0/12/32/32	0/2/2/2
4	SO4	A	1102	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	101	2	-	0/6/23/26	0/1/1/1
4	SO4	B	102	-	-	0/0/0/0	0/0/0/0
3	UDP	C	1101	-	-	0/12/32/32	0/2/2/2
5	NAG	D	101	2	-	0/6/23/26	0/1/1/1
4	SO4	D	102	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	UDP	PB-O2B	-2.05	1.47	1.54
3	C	1101	UDP	C4-N3	2.72	1.38	1.33
3	A	1101	UDP	C4-N3	2.94	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	101	NAG	C1-O5-C5	2.21	115.06	112.25
3	C	1101	UDP	C4-N3-C2	6.52	120.60	114.14
3	A	1101	UDP	C4-N3-C2	6.90	120.97	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	695/723 (96%)	0.50	59 (8%) 13 14	9, 20, 44, 91	0
1	C	674/723 (93%)	0.62	60 (8%) 12 13	10, 19, 47, 119	0
2	B	14/14 (100%)	0.49	2 (14%) 4 4	14, 19, 57, 64	0
2	D	14/14 (100%)	0.48	2 (14%) 4 4	13, 20, 53, 59	0
All	All	1397/1474 (94%)	0.56	123 (8%) 12 13	9, 19, 46, 119	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	VAL	15.8
1	C	339	LEU	15.7
1	C	346	VAL	12.2
1	C	344	LEU	11.8
1	C	347	PHE	11.5
1	C	348	PRO	9.5
1	C	338	ARG	9.5
1	C	340	TYR	9.3
1	C	342	LYS	8.9
1	C	336	ALA	8.9
1	A	718	HIS	8.8
1	C	350	PHE	8.2
1	A	772	ILE	7.8
1	C	718	HIS	7.3
1	A	714	LYS	6.9
1	A	769	MET	6.5
1	A	314	PRO	6.5
1	C	360	VAL	6.4
1	A	713	PHE	5.8
1	C	1028	LYS	5.7
1	C	713	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	343	ALA	5.2
1	A	315	THR	5.2
1	C	746	MET	5.1
1	C	769	MET	4.7
1	A	347	PHE	4.6
1	A	491	ARG	4.5
1	C	714	LYS	4.5
1	A	740	ASP	4.5
1	C	745	LYS	4.4
1	A	745	LYS	4.4
1	C	345	GLU	4.2
1	C	356	ASN	3.9
1	C	740	ASP	3.7
1	C	361	LEU	3.7
1	C	771	THR	3.7
1	A	323	LEU	3.6
1	C	743	ILE	3.6
1	A	331	GLY	3.5
1	A	739	PRO	3.5
1	C	772	ILE	3.4
1	A	768	PRO	3.4
1	C	341	ARG	3.4
1	C	352	ALA	3.4
1	C	742	LYS	3.3
1	A	490	ASN	3.2
1	A	326	ILE	3.2
1	C	770	ASN	3.2
1	A	332	ASN	3.2
1	A	771	THR	3.2
1	A	860	ASN	3.2
1	A	488	GLU	3.2
2	D	26	MET	3.1
1	C	529	HIS	3.0
1	A	534	GLU	3.0
1	A	680	GLU	3.0
1	C	860	ASN	3.0
1	A	335	GLU	3.0
1	C	739	PRO	3.0
1	C	763	ASN	2.9
1	A	770	ASN	2.9
1	A	384	PHE	2.9
1	C	357	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	532	PRO	2.9
1	A	742	LYS	2.8
1	C	712	ASP	2.8
1	A	383	THR	2.8
1	C	363	GLN	2.7
2	B	26	MET	2.7
1	C	383	THR	2.7
1	A	333	ILE	2.6
1	A	507	HIS	2.6
1	A	520	LEU	2.6
1	C	866	LEU	2.6
1	A	743	ILE	2.6
1	A	866	LEU	2.6
1	A	537	LYS	2.6
1	C	359	SER	2.5
1	A	744	VAL	2.5
1	A	329	GLU	2.5
1	C	768	PRO	2.5
2	B	25	MET	2.5
1	A	519	ASN	2.5
1	A	346	VAL	2.5
1	A	526	ASN	2.5
1	C	1020	GLY	2.5
1	C	837	PHE	2.5
1	A	830	ASP	2.4
1	A	489	LYS	2.4
1	C	353	ALA	2.4
1	A	774	GLU	2.4
1	A	609	PRO	2.4
1	C	450	PRO	2.4
1	A	763	ASN	2.4
1	C	526	ASN	2.4
1	C	680	GLU	2.3
2	D	25	MET	2.3
1	A	837	PHE	2.3
1	A	319[A]	SER	2.3
1	A	330	GLN	2.3
1	A	773	ALA	2.3
1	C	744	VAL	2.3
1	A	543	ASP	2.2
1	A	325	ASN	2.2
1	C	519	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	485	ASP	2.2
1	C	774	GLU	2.1
1	A	868	PHE	2.1
1	A	529	HIS	2.1
1	A	327	LYS	2.1
1	C	384	PHE	2.1
1	C	677	GLU	2.1
1	A	318	ASP	2.1
1	A	531	PRO	2.1
1	C	362	GLN	2.1
1	C	364	GLN	2.1
1	A	317	ALA	2.1
1	C	358	ALA	2.1
1	C	773	ALA	2.1
1	C	864	TRP	2.1
1	C	719	ILE	2.1
1	C	884	GLY	2.0
1	A	515[A]	GLU	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](#)

There are no carbohydrates in this entry.

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
4	SO4	D	102	5/5	0.95	0.14	0.85	43,45,48,50	0
4	SO4	B	102	5/5	0.97	0.14	0.70	43,43,47,48	0
5	NAG	B	101	14/15	0.94	0.12	-0.11	12,14,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	D	101	14/15	0.95	0.12	-0.18	11,14,17,19	0
3	UDP	A	1101	25/25	0.98	0.12	-0.99	8,10,13,15	0
3	UDP	C	1101	25/25	0.98	0.11	-1.09	9,11,13,15	0
4	SO4	A	1102	5/5	0.91	0.16	-	57,57,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.