



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:19 PM GMT

PDB ID : 4EE4
Title : Crystal structure of human M340H-beta-1,4-galactosyltransferase-1 (M340H-B4GAL-T1) in complex with tetrasaccharide from Lacto-N-neohexose
Authors : Ramakrishnan, B.; Qasba, P.K.
Deposited on : 2012-03-28
Resolution : 1.95 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

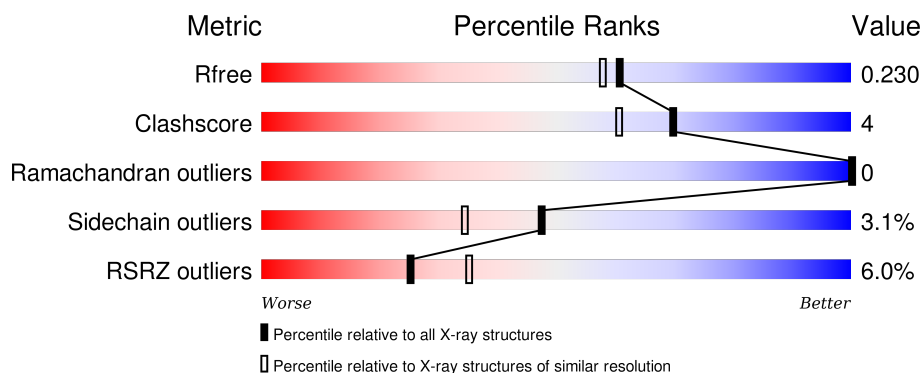
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	287	<div> <div>3%</div> <div>83% 12% • 5%</div> </div>
1	B	287	<div> <div>7%</div> <div>85% 8% • 5%</div> </div>
1	C	287	<div> <div>7%</div> <div>84% 11% • 5%</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
5	SO4	A	410	-	-	-	X
5	SO4	A	411	-	-	-	X
5	SO4	A	413	-	-	-	X
5	SO4	B	409	-	-	-	X
5	SO4	B	413	-	-	-	X
5	SO4	B	414	-	-	-	X
5	SO4	B	417	-	-	-	X
5	SO4	C	407	-	-	-	X
5	SO4	C	409	-	-	-	X
6	GOL	A	414	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7755 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-1,4-galactosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	3	0
			2233	1430	387	405	11			
1	B	273	Total	C	N	O	S	0	4	0
			2238	1433	386	408	11			
1	C	273	Total	C	N	O	S	0	1	0
			2224	1424	387	402	11			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	-	EXPRESSION TAG	UNP P15291
A	113	SER	-	EXPRESSION TAG	UNP P15291
A	114	MET	-	EXPRESSION TAG	UNP P15291
A	115	THR	-	EXPRESSION TAG	UNP P15291
A	116	GLY	-	EXPRESSION TAG	UNP P15291
A	117	GLY	-	EXPRESSION TAG	UNP P15291
A	118	GLN	-	EXPRESSION TAG	UNP P15291
A	119	GLN	-	EXPRESSION TAG	UNP P15291
A	120	MET	-	EXPRESSION TAG	UNP P15291
A	121	GLY	-	EXPRESSION TAG	UNP P15291
A	122	ARG	-	EXPRESSION TAG	UNP P15291
A	123	GLY	-	EXPRESSION TAG	UNP P15291
A	124	SER	-	EXPRESSION TAG	UNP P15291
A	125	ALA	-	EXPRESSION TAG	UNP P15291
A	337	THR	ARG	ENGINEERED MUTATION	UNP P15291
A	338	THR	CYS	ENGINEERED MUTATION	UNP P15291
A	340	HIS	MET	ENGINEERED MUTATION	UNP P15291
B	112	ALA	-	EXPRESSION TAG	UNP P15291
B	113	SER	-	EXPRESSION TAG	UNP P15291
B	114	MET	-	EXPRESSION TAG	UNP P15291
B	115	THR	-	EXPRESSION TAG	UNP P15291
B	116	GLY	-	EXPRESSION TAG	UNP P15291
B	117	GLY	-	EXPRESSION TAG	UNP P15291

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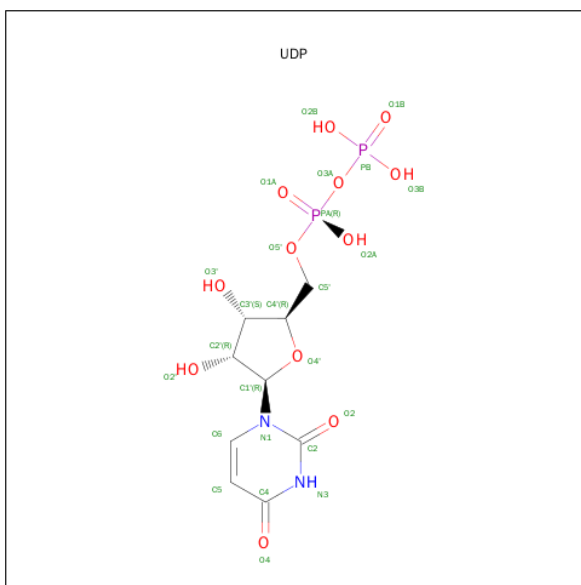
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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLN	-	EXPRESSION TAG	UNP P15291
B	119	GLN	-	EXPRESSION TAG	UNP P15291
B	120	MET	-	EXPRESSION TAG	UNP P15291
B	121	GLY	-	EXPRESSION TAG	UNP P15291
B	122	ARG	-	EXPRESSION TAG	UNP P15291
B	123	GLY	-	EXPRESSION TAG	UNP P15291
B	124	SER	-	EXPRESSION TAG	UNP P15291
B	125	ALA	-	EXPRESSION TAG	UNP P15291
B	337	THR	ARG	ENGINEERED MUTATION	UNP P15291
B	338	THR	CYS	ENGINEERED MUTATION	UNP P15291
B	340	HIS	MET	ENGINEERED MUTATION	UNP P15291
C	112	ALA	-	EXPRESSION TAG	UNP P15291
C	113	SER	-	EXPRESSION TAG	UNP P15291
C	114	MET	-	EXPRESSION TAG	UNP P15291
C	115	THR	-	EXPRESSION TAG	UNP P15291
C	116	GLY	-	EXPRESSION TAG	UNP P15291
C	117	GLY	-	EXPRESSION TAG	UNP P15291
C	118	GLN	-	EXPRESSION TAG	UNP P15291
C	119	GLN	-	EXPRESSION TAG	UNP P15291
C	120	MET	-	EXPRESSION TAG	UNP P15291
C	121	GLY	-	EXPRESSION TAG	UNP P15291
C	122	ARG	-	EXPRESSION TAG	UNP P15291
C	123	GLY	-	EXPRESSION TAG	UNP P15291
C	124	SER	-	EXPRESSION TAG	UNP P15291
C	125	ALA	-	EXPRESSION TAG	UNP P15291
C	337	THR	ARG	ENGINEERED MUTATION	UNP P15291
C	338	THR	CYS	ENGINEERED MUTATION	UNP P15291
C	340	HIS	MET	ENGINEERED MUTATION	UNP P15291

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			51	28	2	21		
2	B	4	Total	C	N	O	0	0
			51	28	2	21		
2	C	4	Total	C	N	O	0	0
			51	28	2	21		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).

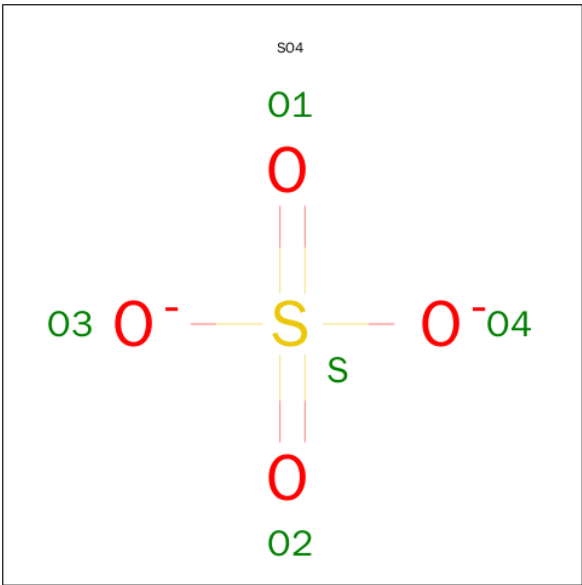


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



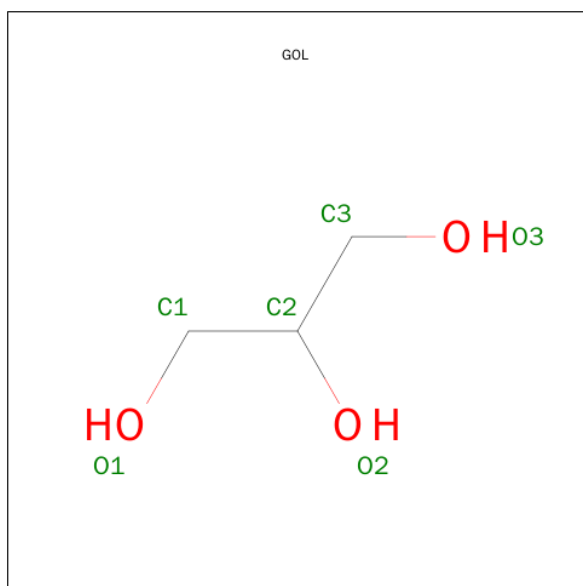
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

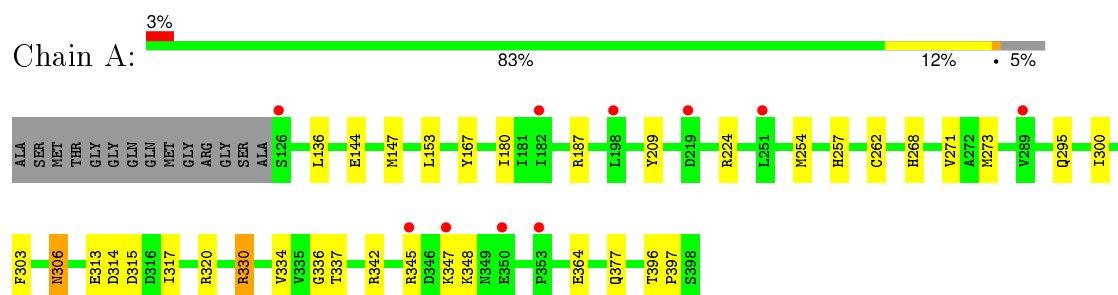
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	246	Total	O	0	0
			246	246		
7	B	269	Total	O	0	0
			269	269		
7	C	180	Total	O	0	0
			180	180		

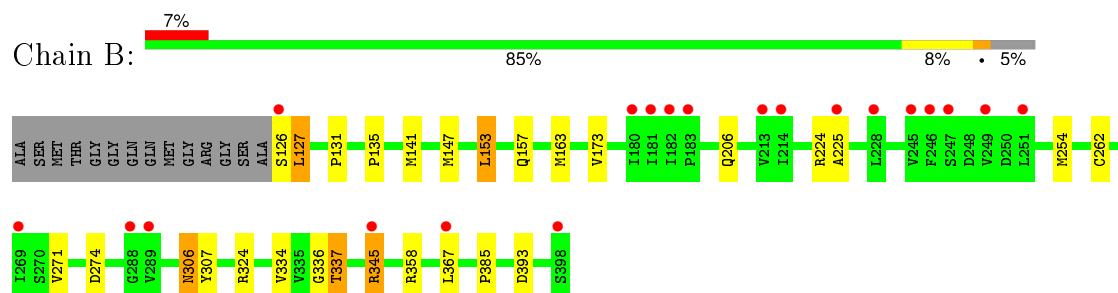
3 Residue-property plots [i](#)

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.

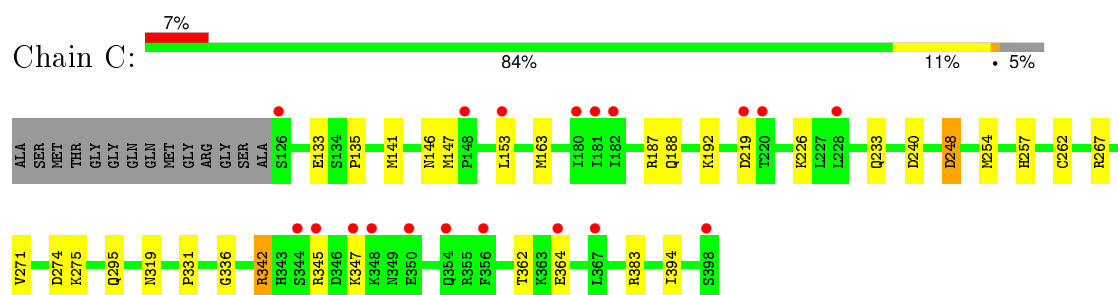
• Molecule 1: Beta-1,4-galactosyltransferase 1



• Molecule 1: Beta-1,4-galactosyltransferase 1



• Molecule 1: Beta-1,4-galactosyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.36Å 195.97Å 143.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.82 – 1.95 36.82 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.0 (36.82-1.95) 93.1 (36.82-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.195 , 0.232 0.194 , 0.230	Depositor DCC
R_{free} test set	5495 reflections (5.65%)	DCC
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.4	EDS
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.009 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 102441 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7755	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: GOL, UDP, BGC, NAG, MN, GAL, 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	0.98	0/2304	0.96	8/3130 (0.3%)
1	B	1.02	1/2312 (0.0%)	0.99	5/3141 (0.2%)
1	C	0.79	0/2289	0.84	2/3109 (0.1%)
All	All	0.93	1/6905 (0.0%)	0.94	15/9380 (0.2%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	ALA	CA-CB	5.36	1.63	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	CYS	CA-CB-SG	-7.81	99.94	114.00
1	A	187	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	262	CYS	CA-CB-SG	-7.38	100.72	114.00
1	B	224	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	C	262	CYS	CA-CB-SG	-5.63	103.86	114.00
1	A	187	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	274	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	315	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	393	ASP	CB-CG-OD2	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	141	MET	CG-SD-CE	5.21	108.53	100.20
1	C	248	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	330	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	180	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	A	273	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	126	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2233	0	2181	24	0
1	B	2238	0	2183	19	0
1	C	2224	0	2170	20	0
2	A	51	0	45	0	0
2	B	51	0	45	0	0
2	C	51	0	45	1	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
3	C	25	0	11	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	35	0	0	1	0
5	B	55	0	0	0	0
5	C	20	0	0	1	0
6	A	6	0	8	0	0
6	B	12	0	15	0	0
6	C	6	0	8	1	0
7	A	246	0	0	4	0
7	B	269	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	180	0	0	5	0
All	All	7755	0	6733	62	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 4.

All (62) 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:306:ASN:HD22	1:A:306:ASN:H	1.26	0.80
1:A:254:MET:SD	1:A:337[A]:THR:HG22	2.23	0.78
1:A:377:GLN:HG2	7:A:722:HOH:O	1.83	0.78
1:A:334:VAL:O	1:A:337[B]:THR:HG23	1.83	0.77
1:B:334:VAL:O	1:B:337[B]:THR:HG23	1.87	0.74
1:B:337[B]:THR:HG21	1:C:135:PRO:HB2	1.68	0.74
1:B:254:MET:SD	1:B:337[A]:THR:CG2	2.78	0.71
3:C:405:UDP:H3'	3:C:405:UDP:O1A	1.93	0.69
1:B:306:ASN:HD22	1:B:306:ASN:H	1.40	0.69
1:A:254:MET:SD	1:A:337[A]:THR:CG2	2.80	0.69
1:C:141:MET:SD	7:C:611:HOH:O	2.52	0.68
1:C:240:ASP:HB2	7:C:577:HOH:O	1.92	0.68
1:C:342:ARG:NH2	7:C:607:HOH:O	2.25	0.63
1:A:295:GLN:HG2	7:A:662:HOH:O	2.00	0.62
1:A:337[B]:THR:HG21	1:B:135:PRO:HB2	1.83	0.61
1:B:131:PRO:HD2	1:B:206:GLN:HE22	1.71	0.56
1:A:306:ASN:N	1:A:306:ASN:HD22	1.93	0.55
1:A:257:HIS:HE1	7:A:665:HOH:O	1.89	0.55
1:C:226:LYS:NZ	1:C:394:ILE:O	2.37	0.54
1:B:254:MET:CG	1:B:337[A]:THR:HG22	2.38	0.54
1:B:306:ASN:ND2	1:B:306:ASN:H	2.03	0.54
1:A:377:GLN:CG	7:A:722:HOH:O	2.48	0.53
1:A:306:ASN:H	1:A:306:ASN:ND2	2.01	0.52
1:B:254:MET:SD	1:B:337[A]:THR:HG22	2.51	0.51
1:C:267:ARG:NH2	5:C:409:SO4:O1	2.43	0.50
2:C:403:NAG:O4	6:C:411:GOL:H32	2.12	0.49
1:C:187:ARG:NH2	3:C:405:UDP:O1A	2.41	0.49
1:C:240:ASP:CB	7:C:577:HOH:O	2.53	0.48
1:C:248:ASP:HB3	3:C:405:UDP:O3'	2.12	0.48
1:A:144:GLU:HA	5:A:407:SO4:O3	2.12	0.48
1:B:271:VAL:HG22	1:B:336:GLY:HA3	1.97	0.47
1:A:306:ASN:N	1:A:306:ASN:ND2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:MET:CE	1:C:383:ARG:O	2.63	0.47
1:C:254:MET:HE3	1:C:254:MET:HB3	1.60	0.46
1:C:342:ARG:HA	1:C:342:ARG:NE	2.30	0.46
1:B:254:MET:SD	1:B:337[A]:THR:HG21	2.54	0.46
1:B:306:ASN:HD22	1:B:306:ASN:N	2.04	0.46
1:B:306:ASN:ND2	1:B:306:ASN:N	2.64	0.45
1:B:153:LEU:HD12	1:B:157:GLN:NE2	2.31	0.45
1:A:396:THR:HB	1:A:397:PRO:HD2	1.99	0.45
1:C:274:ASP:OD1	1:C:275:LYS:N	2.50	0.45
1:A:136:LEU:HA	1:C:254:MET:HE1	2.00	0.44
1:C:188:GLN:O	1:C:192:LYS:HG3	2.18	0.43
1:C:319:ASN:HB2	1:C:362:THR:HG21	1.99	0.43
1:B:127:LEU:HB3	1:B:173:VAL:HG23	2.01	0.43
1:A:224:ARG:HD3	1:A:313:GLU:OE1	2.20	0.42
1:A:314:ASP:N	1:A:314:ASP:OD1	2.52	0.42
1:B:324:ARG:HH22	1:B:367:LEU:HD21	1.84	0.42
1:B:345:ARG:NH1	7:B:524:HOH:O	2.52	0.41
1:C:271:VAL:HG22	1:C:336:GLY:HA3	2.01	0.41
1:A:268:HIS:HB3	1:A:330:ARG:HG2	2.02	0.41
1:C:146:ASN:OD1	7:C:585:HOH:O	2.22	0.41
1:A:303:PHE:CD1	1:A:317:ILE:HG12	2.55	0.41
1:C:342:ARG:HA	1:C:342:ARG:HE	1.86	0.41
1:B:307:TYR:CZ	1:B:358:ARG:HB3	2.56	0.41
1:A:271:VAL:HG22	1:A:336:GLY:HA3	2.03	0.41
1:A:330:ARG:HD2	1:A:330:ARG:HH11	1.70	0.41
1:C:271:VAL:HG11	1:C:331:PRO:HD2	2.02	0.40
1:A:167:TYR:HB3	1:A:209:TYR:CE2	2.56	0.40
1:A:347:LYS:O	1:A:348:LYS:HB2	2.21	0.40
1:A:300:ILE:HB	1:A:320:ARG:HB3	2.04	0.40
1:B:163:MET:HE2	7:B:659:HOH:O	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	274/287 (96%)	268 (98%)	6 (2%)	0	100	100
1	B	275/287 (96%)	272 (99%)	3 (1%)	0	100	100
1	C	272/287 (95%)	263 (97%)	9 (3%)	0	100	100
All	All	821/861 (95%)	803 (98%)	18 (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	247/252 (98%)	242 (98%)	5 (2%)	63	55
1	B	248/252 (98%)	240 (97%)	8 (3%)	46	33
1	C	245/252 (97%)	233 (95%)	12 (5%)	31	15
All	All	740/756 (98%)	715 (97%)	25 (3%)	47	30

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	MET
1	A	153	LEU
1	A	306	ASN
1	A	345	ARG
1	A	364	GLU
1	B	127	LEU
1	B	147	MET
1	B	153	LEU
1	B	306	ASN
1	B	337[A]	THR
1	B	337[B]	THR
1	B	345	ARG
1	B	385	PRO

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Mol	Chain	Res	Type
1	C	133	GLU
1	C	147	MET
1	C	153	LEU
1	C	219	ASP
1	C	233	GLN
1	C	257	HIS
1	C	295[A]	GLN
1	C	295[B]	GLN
1	C	342	ARG
1	C	345	ARG
1	C	347	LYS
1	C	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	257	HIS
1	A	306	ASN
1	B	157	GLN
1	B	186	ASN
1	B	206	GLN
1	B	306	ASN
1	C	206	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 ⓘ

12 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	BGC	A	401	2	12,12,12	0.87	0	17,17,17	1.26	2 (11%)
2	GAL	A	402	2	11,11,12	0.67	0	14,15,17	1.45	2 (14%)
2	NAG	A	403	2	14,14,15	0.57	0	15,19,21	0.92	1 (6%)
2	NAG	A	404	2	14,14,15	0.54	0	15,19,21	1.90	5 (33%)
2	BGC	B	401	2	12,12,12	0.64	0	17,17,17	1.42	2 (11%)
2	GAL	B	402	2	11,11,12	0.66	0	14,15,17	1.32	1 (7%)
2	NAG	B	403	2	14,14,15	0.63	0	15,19,21	1.07	1 (6%)
2	NAG	B	404	2	14,14,15	0.85	0	15,19,21	1.76	5 (33%)
2	BGC	C	401	2	12,12,12	0.67	0	17,17,17	1.74	4 (23%)
2	GAL	C	402	2	11,11,12	0.57	0	14,15,17	1.39	3 (21%)
2	NAG	C	403	2	14,14,15	0.60	0	15,19,21	1.06	1 (6%)
2	NAG	C	404	2	14,14,15	0.62	0	15,19,21	1.56	3 (20%)

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	BGC	A	401	2	-	0/2/22/22	0/1/1/1
2	GAL	A	402	2	-	0/2/19/22	0/1/1/1
2	NAG	A	403	2	-	0/6/23/26	0/1/1/1
2	NAG	A	404	2	-	0/6/23/26	0/1/1/1
2	BGC	B	401	2	-	0/2/22/22	0/1/1/1
2	GAL	B	402	2	-	0/2/19/22	0/1/1/1
2	NAG	B	403	2	-	0/6/23/26	0/1/1/1
2	NAG	B	404	2	-	0/6/23/26	0/1/1/1
2	BGC	C	401	2	-	0/2/22/22	0/1/1/1
2	GAL	C	402	2	-	0/2/19/22	0/1/1/1
2	NAG	C	403	2	-	0/6/23/26	0/1/1/1
2	NAG	C	404	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	BGC	C1-C2-C3	-3.87	104.67	110.43
2	B	401	BGC	C1-O5-C5	-3.18	107.59	113.47
2	C	404	NAG	C6-C5-C4	-3.14	105.27	113.02
2	B	402	GAL	O5-C1-C2	-3.06	105.89	110.86
2	B	404	NAG	C6-C5-C4	-3.06	105.47	113.02
2	C	402	GAL	C2-C3-C4	-2.89	106.13	111.04
2	A	404	NAG	C6-C5-C4	-2.77	106.17	113.02
2	B	403	NAG	C2-N2-C7	-2.69	119.58	123.04
2	A	402	GAL	C2-C3-C4	-2.50	106.79	111.04
2	C	403	NAG	C2-N2-C7	-2.50	119.82	123.04
2	C	401	BGC	C1-O5-C5	-2.50	108.84	113.47
2	B	404	NAG	O3-C3-C4	-2.42	104.89	110.34
2	C	404	NAG	C4-C3-C2	-2.36	107.56	111.23
2	A	404	NAG	C8-C7-N2	-2.30	111.71	116.11
2	B	401	BGC	O4-C4-C3	-2.28	105.20	110.34
2	C	401	BGC	O5-C1-C2	-2.25	106.22	109.80
2	A	401	BGC	O5-C5-C6	-2.13	100.98	106.36
2	A	403	NAG	C3-C4-C5	-2.09	106.56	110.20
2	A	401	BGC	O2-C2-C1	-2.05	105.30	109.82
2	C	402	GAL	O3-C3-C2	-2.04	106.32	110.00
2	A	404	NAG	C1-O5-C5	2.05	114.85	112.25
2	C	401	BGC	O3-C3-C2	2.13	115.14	110.34
2	C	402	GAL	C1-C2-C3	2.25	112.21	109.54
2	B	404	NAG	O7-C7-N2	2.30	126.56	121.86
2	C	404	NAG	O5-C5-C6	2.59	112.96	107.35
2	B	404	NAG	C1-O5-C5	2.59	115.54	112.25
2	A	404	NAG	O7-C7-N2	2.69	127.35	121.86
2	B	404	NAG	C2-N2-C7	3.33	127.32	123.04
2	A	402	GAL	C1-C2-C3	3.90	114.15	109.54
2	A	404	NAG	C2-N2-C7	4.49	128.81	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	NAG	1	0

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 3 are monoatomic - leaving 29 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	$\# Z > 2$
3	UDP	A	405	4	18,26,26	1.59	3 (16%)	26,40,40	1.96	3 (11%)
5	SO4	A	407	-	4,4,4	0.22	0	6,6,6	0.79	0
5	SO4	A	408	-	4,4,4	0.27	0	6,6,6	0.71	0
5	SO4	A	409	-	4,4,4	0.17	0	6,6,6	0.51	0
5	SO4	A	410	-	4,4,4	0.33	0	6,6,6	1.11	1 (16%)
5	SO4	A	411	-	4,4,4	0.24	0	6,6,6	0.28	0
5	SO4	A	412	-	4,4,4	0.15	0	6,6,6	0.48	0
5	SO4	A	413	-	4,4,4	0.21	0	6,6,6	0.62	0
6	GOL	A	414	-	5,5,5	0.45	0	5,5,5	1.09	0
3	UDP	B	405	4	18,26,26	1.46	3 (16%)	26,40,40	1.37	5 (19%)
5	SO4	B	407	-	4,4,4	0.21	0	6,6,6	0.28	0
5	SO4	B	408	-	4,4,4	0.13	0	6,6,6	0.67	0
5	SO4	B	409	-	4,4,4	0.48	0	6,6,6	0.94	1 (16%)
5	SO4	B	410	-	4,4,4	0.30	0	6,6,6	0.35	0
5	SO4	B	411	-	4,4,4	0.16	0	6,6,6	0.41	0
5	SO4	B	412	-	4,4,4	0.23	0	6,6,6	0.57	0
5	SO4	B	413	-	4,4,4	0.51	0	6,6,6	0.63	0
5	SO4	B	414	-	4,4,4	0.17	0	6,6,6	0.53	0
5	SO4	B	415	-	4,4,4	0.11	0	6,6,6	0.30	0
5	SO4	B	416	-	4,4,4	0.10	0	6,6,6	0.29	0
5	SO4	B	417	-	4,4,4	0.21	0	6,6,6	0.20	0
6	GOL	B	418	-	5,5,5	0.20	0	5,5,5	2.01	2 (40%)
6	GOL	B	419	-	5,5,5	0.45	0	5,5,5	0.94	0
3	UDP	C	405	4	18,26,26	1.11	1 (5%)	26,40,40	1.65	4 (15%)
5	SO4	C	407	-	4,4,4	0.30	0	6,6,6	0.62	0
5	SO4	C	408	-	4,4,4	0.13	0	6,6,6	0.21	0
5	SO4	C	409	-	4,4,4	0.17	0	6,6,6	0.56	0
5	SO4	C	410	-	4,4,4	0.16	0	6,6,6	0.12	0
6	GOL	C	411	-	5,5,5	0.29	0	5,5,5	1.15	1 (20%)

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	405	4	-	0/12/32/32	0/2/2/2
5	SO4	A	407	-	-	0/0/0/0	0/0/0/0
5	SO4	A	408	-	-	0/0/0/0	0/0/0/0
5	SO4	A	409	-	-	0/0/0/0	0/0/0/0
5	SO4	A	410	-	-	0/0/0/0	0/0/0/0
5	SO4	A	411	-	-	0/0/0/0	0/0/0/0
5	SO4	A	412	-	-	0/0/0/0	0/0/0/0
5	SO4	A	413	-	-	0/0/0/0	0/0/0/0
6	GOL	A	414	-	-	0/4/4/4	0/0/0/0
3	UDP	B	405	4	-	0/12/32/32	0/2/2/2
5	SO4	B	407	-	-	0/0/0/0	0/0/0/0
5	SO4	B	408	-	-	0/0/0/0	0/0/0/0
5	SO4	B	409	-	-	0/0/0/0	0/0/0/0
5	SO4	B	410	-	-	0/0/0/0	0/0/0/0
5	SO4	B	411	-	-	0/0/0/0	0/0/0/0
5	SO4	B	412	-	-	0/0/0/0	0/0/0/0
5	SO4	B	413	-	-	0/0/0/0	0/0/0/0
5	SO4	B	414	-	-	0/0/0/0	0/0/0/0
5	SO4	B	415	-	-	0/0/0/0	0/0/0/0
5	SO4	B	416	-	-	0/0/0/0	0/0/0/0
5	SO4	B	417	-	-	0/0/0/0	0/0/0/0
6	GOL	B	418	-	-	0/4/4/4	0/0/0/0
6	GOL	B	419	-	-	0/4/4/4	0/0/0/0
3	UDP	C	405	4	-	0/12/32/32	0/2/2/2
5	SO4	C	407	-	-	0/0/0/0	0/0/0/0
5	SO4	C	408	-	-	0/0/0/0	0/0/0/0
5	SO4	C	409	-	-	0/0/0/0	0/0/0/0
5	SO4	C	410	-	-	0/0/0/0	0/0/0/0
6	GOL	C	411	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	405	UDP	C6-N1	2.11	1.38	1.35
3	A	405	UDP	C6-C5	2.28	1.43	1.38
3	B	405	UDP	O4'-C1'	2.89	1.44	1.41
3	C	405	UDP	C4-N3	3.13	1.38	1.33
3	A	405	UDP	C4-N3	3.26	1.39	1.33
3	B	405	UDP	C4-N3	3.56	1.39	1.33
3	A	405	UDP	C6-N1	3.89	1.41	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	405	UDP	C6-N1-C2	-2.48	117.26	121.28
6	C	411	GOL	C3-C2-C1	-2.38	101.80	111.12
3	B	405	UDP	PA-O3A-PB	-2.29	125.00	132.67
3	C	405	UDP	PA-O3A-PB	-2.09	125.64	132.67
5	B	409	SO4	O4-S-O3	-2.03	100.71	108.98
3	B	405	UDP	O3B-PB-O3A	2.00	114.17	105.09
3	B	405	UDP	O4'-C1'-N1	2.38	113.10	108.08
3	A	405	UDP	O3A-PA-O5'	2.43	109.38	102.94
5	A	410	SO4	O2-S-O1	2.44	117.24	109.50
6	B	418	GOL	O2-C2-C3	2.72	121.14	108.65
3	A	405	UDP	O5'-C5'-C4'	2.73	119.19	109.12
3	B	405	UDP	C4-N3-C2	2.87	116.99	114.14
3	C	405	UDP	O4'-C1'-N1	2.96	114.33	108.08
6	B	418	GOL	O2-C2-C1	3.38	124.14	108.65
3	B	405	UDP	O3A-PA-O5'	3.46	112.11	102.94
3	C	405	UDP	C4-N3-C2	5.59	119.67	114.14
3	A	405	UDP	C4-N3-C2	8.00	122.07	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	SO4	1	0
3	C	405	UDP	3	0
5	C	409	SO4	1	0
6	C	411	GOL	1	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	273/287 (95%)	0.16	10 (3%) 45 56	22, 31, 49, 70	0
1	B	273/287 (95%)	0.29	20 (7%) 18 28	21, 27, 42, 61	0
1	C	273/287 (95%)	0.42	19 (6%) 19 29	28, 39, 58, 72	0
All	All	819/861 (95%)	0.29	49 (5%) 25 35	21, 33, 54, 72	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	SER	5.4
1	C	347	LYS	5.2
1	B	126	SER	4.7
1	C	153	LEU	4.3
1	B	182	ILE	4.2
1	C	398	SER	4.1
1	B	228	LEU	4.1
1	B	181	ILE	3.8
1	C	126	SER	3.7
1	B	398	SER	3.7
1	A	347	LYS	3.5
1	B	214	ILE	3.4
1	B	289	VAL	3.4
1	C	345	ARG	3.2
1	C	364	GLU	3.2
1	A	345	ARG	3.1
1	C	148	PRO	3.1
1	B	246	PHE	2.8
1	C	350	GLU	2.7
1	A	251	LEU	2.7
1	C	344	SER	2.7
1	C	181	ILE	2.7
1	A	350	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	249	VAL	2.6
1	B	183	PRO	2.6
1	B	251	LEU	2.6
1	A	289	VAL	2.6
1	B	213	VAL	2.6
1	A	219	ASP	2.6
1	B	367	LEU	2.5
1	C	220	THR	2.5
1	A	198	LEU	2.5
1	C	182	ILE	2.4
1	C	219	ASP	2.2
1	B	245	VAL	2.2
1	B	180	ILE	2.2
1	C	180	ILE	2.2
1	C	228	LEU	2.2
1	C	356	PHE	2.1
1	C	348	LYS	2.1
1	B	345	ARG	2.1
1	B	247	SER	2.1
1	B	269	ILE	2.1
1	A	353	PRO	2.1
1	C	354	GLN	2.1
1	C	367	LEU	2.1
1	B	288	GLY	2.0
1	B	225	ALA	2.0
1	A	182	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	403	14/15	0.97	0.10	-0.34	23,26,29,29	0
2	NAG	C	403	14/15	0.95	0.07	-1.48	43,45,46,47	0
2	NAG	A	403	14/15	0.98	0.06	-2.35	26,30,32,32	0
2	BGC	C	401	12/12	0.92	0.19	-	55,59,65,66	0
2	NAG	A	404	14/15	0.93	0.20	-	51,57,60,62	0
2	GAL	B	402	11/12	0.98	0.09	-	31,35,40,43	0
2	NAG	C	404	14/15	0.91	0.23	-	59,66,68,71	0
2	BGC	B	401	12/12	0.92	0.14	-	34,44,54,55	0
2	NAG	B	404	14/15	0.96	0.16	-	40,48,50,58	0
2	GAL	A	402	11/12	0.96	0.13	-	32,38,49,50	0
2	GAL	C	402	11/12	0.94	0.13	-	50,55,57,58	0
2	BGC	A	401	12/12	0.95	0.11	-	36,41,52,56	0

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	C	409	5/5	0.75	0.35	9.19	91,92,92,94	0
5	SO4	A	413	5/5	0.85	0.45	8.16	126,127,128,128	0
5	SO4	A	411	5/5	0.83	0.22	4.82	83,84,87,89	0
5	SO4	A	410	5/5	0.75	0.23	4.76	76,85,86,87	0
5	SO4	B	413	5/5	0.93	0.29	4.42	45,53,59,60	0
5	SO4	B	417	5/5	0.83	0.38	4.40	122,122,123,123	0
5	SO4	B	414	5/5	0.68	0.30	3.61	101,105,107,108	0
6	GOL	A	414	6/6	0.88	0.20	3.29	32,41,51,59	0
5	SO4	C	407	5/5	0.97	0.15	2.21	47,50,52,58	0
5	SO4	B	409	5/5	0.79	0.28	2.13	66,74,74,77	0
6	GOL	C	411	6/6	0.88	0.19	1.93	45,55,56,61	0
5	SO4	A	408	5/5	0.90	0.18	1.68	58,64,66,69	0
6	GOL	B	418	6/6	0.93	0.18	0.87	28,39,49,53	0
3	UDP	B	405	25/25	0.83	0.20	0.70	23,29,98,101	0
5	SO4	C	408	5/5	0.90	0.15	0.60	80,81,84,84	0
3	UDP	A	405	25/25	0.80	0.19	0.53	30,41,109,109	0
3	UDP	C	405	25/25	0.80	0.22	0.52	41,49,117,118	0
5	SO4	A	407	5/5	0.91	0.11	-0.72	72,73,75,76	0
5	SO4	B	408	5/5	0.97	0.09	-1.45	62,65,65,65	0
6	GOL	B	419	6/6	0.97	0.09	-1.52	26,30,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	412	5/5	0.72	0.28	-	107,107,108,109	0
5	SO4	B	411	5/5	0.89	0.26	-	75,76,77,79	0
5	SO4	B	416	5/5	0.49	0.41	-	121,122,123,123	0
5	SO4	B	415	5/5	0.86	0.44	-	94,94,96,97	0
4	MN	A	406	1/1	0.95	0.04	-	59,59,59,59	0
5	SO4	B	412	5/5	0.70	0.29	-	105,105,107,107	0
5	SO4	A	409	5/5	0.86	0.35	-	73,75,78,80	0
4	MN	B	406	1/1	1.00	0.06	-	45,45,45,45	0
5	SO4	C	410	5/5	0.90	0.26	-	100,101,102,103	0
5	SO4	B	407	5/5	0.96	0.21	-	82,82,84,85	0
4	MN	C	406	1/1	0.93	0.10	-	64,64,64,64	0
5	SO4	B	410	5/5	0.54	0.34	-	101,105,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.