



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 AM GMT

PDB ID : 2X61  
Title : CRYSTAL STRUCTURE OF THE SIALYLTRANSFERASE CST-II IN  
COMPLEX WITH TRISACCHARIDE ACCEPTOR AND CMP  
Authors : Lee, H.J.; Lairson, L.L.; Rich, J.R.; Wakarchuk, W.W.; Withers, S.G.; Stry-  
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Deposited on : 2010-02-16  
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](mailto: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.

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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

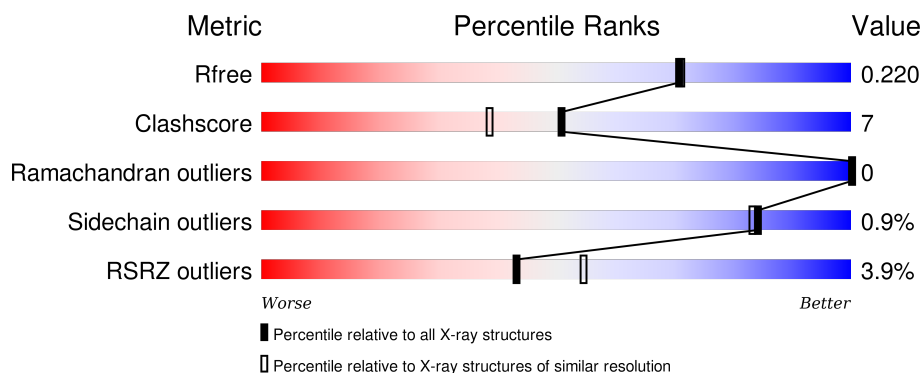
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

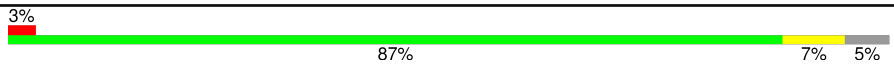

The reported resolution of this entry is 1.95 Å.

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  $\geq 3$ , 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	258	
1	B	258	

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	SIA	A	1261	X	-	-	-
2	SIA	B	1261	X	-	-	-
4	MPD	A	1263	-	-	X	X
6	EDO	B	1263	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4512 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 ALPHA-2,3-/2,8-SIALYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	2	0
			2057	1353	321	375	8			
1	B	243	Total	C	N	O	S	0	0	0
			2030	1334	317	371	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	SER	ILE	ENGINEERED MUTATION	UNP Q9LAK3
A	222	GLY	GLU	ENGINEERED MUTATION	UNP Q9LAK3
B	53	SER	ILE	ENGINEERED MUTATION	UNP Q9LAK3
B	222	GLY	GLU	ENGINEERED MUTATION	UNP Q9LAK3

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

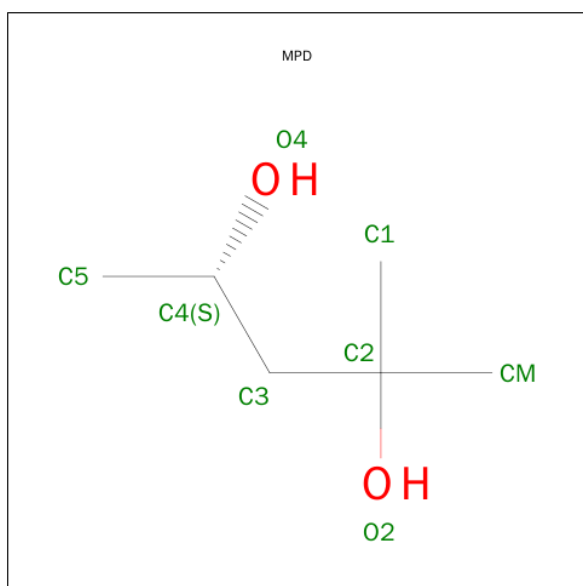
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			46	25	2	19		
2	B	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



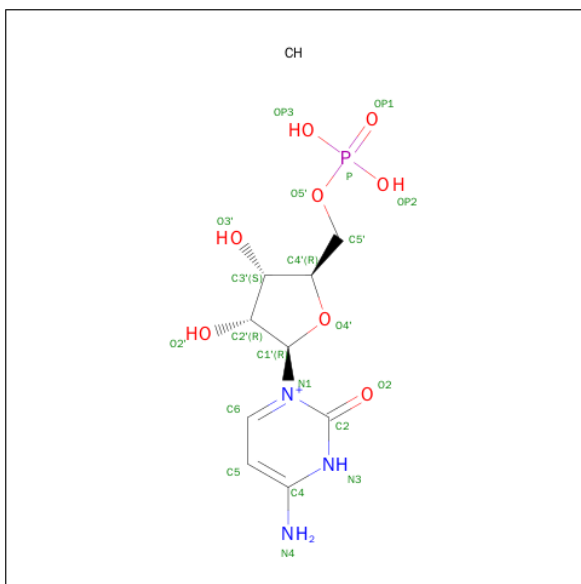
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is N3-PROTONATED CYTIDINE-5'-MONOPHOSPHATE (three-letter code: CH) (formula:  $C_9H_{15}N_3O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
5	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

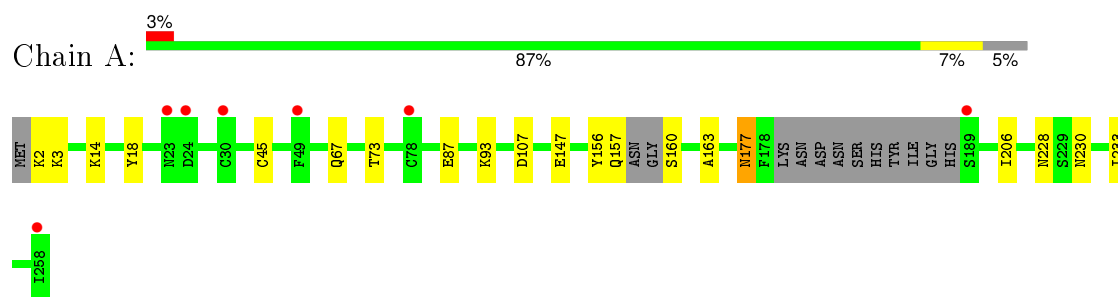
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	162	Total	O	0	0
			162	162		
7	B	101	Total	O	0	0
			101	101		

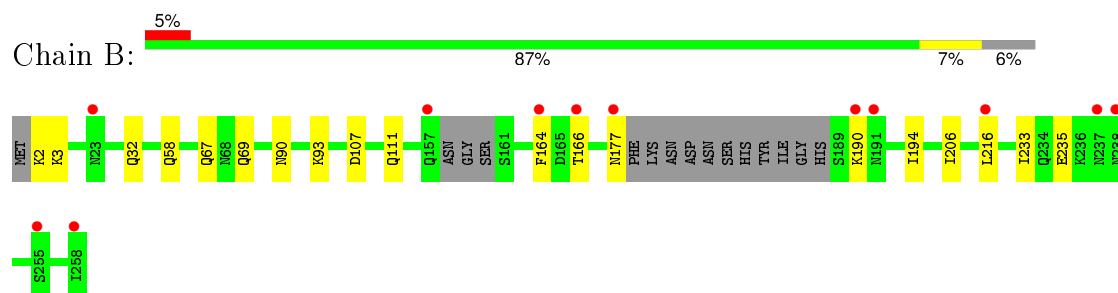
### 3 Residue-property plots [i](#)

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: ALPHA-2,3-/2,8-SIALYLTRANSFERASE



- Molecule 1: ALPHA-2,3-/2,8-SIALYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.67Å 117.67Å 46.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 36.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.95) 99.6 (36.53-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.164 , 0.198 0.183 , 0.220	Depositor DCC
$R_{free}$ test set	2368 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.3	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 46776 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, CH, NGA, EDO, SIA, GAL, ACT

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	0.44	0/2119	0.51	0/2856
1	B	0.40	0/2084	0.48	0/2809
All	All	0.42	0/4203	0.50	0/5665

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
2	A	1	0
2	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1261	SIA	C8
2	B	1261	SIA	C8

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	2057	0	2002	23	0
1	B	2030	0	1976	22	0
2	A	46	0	38	2	0
2	B	46	0	38	0	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	8	0	14	9	0
5	A	21	0	13	0	0
5	B	21	0	13	5	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	A	162	0	0	13	0
7	B	101	0	0	4	0
All	All	4512	0	4115	58	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 7.

All (58) 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)
4:A:1263:MPD:H12	4:A:1263:MPD:C5	1.55	1.27
1:A:93:LYS:HE2	7:A:2065:HOH:O	1.38	1.22
1:A:2:LYS:HG2	1:A:3:LYS:H	1.09	1.17
4:A:1263:MPD:H53	4:A:1263:MPD:C1	1.77	1.13
5:B:1262:CH:H5'	5:B:1262:CH:H6	1.22	1.12
1:A:93:LYS:CE	7:A:2065:HOH:O	1.98	1.06
5:B:1262:CH:C5'	5:B:1262:CH:H6	1.88	1.04
1:B:2:LYS:HG2	1:B:3:LYS:N	1.69	1.01
1:A:107:ASP:OD1	7:A:2082:HOH:O	1.78	1.01
4:A:1263:MPD:H4	7:A:2078:HOH:O	1.58	1.00
1:B:2:LYS:HG2	1:B:3:LYS:H	0.87	1.00
1:B:2:LYS:CG	1:B:3:LYS:H	1.79	0.90
1:A:2:LYS:HG2	1:A:3:LYS:N	1.87	0.89
5:B:1262:CH:H5'	5:B:1262:CH:C6	2.02	0.89
1:A:160:SER:CB	1:B:67:GLN:OE1	2.24	0.86
4:A:1263:MPD:H12	4:A:1263:MPD:H53	0.87	0.84
1:A:3:LYS:NZ	1:A:147:GLU:OE1	2.10	0.84
4:A:1263:MPD:C5	4:A:1263:MPD:C1	2.35	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:HB2	1:B:67:GLN:OE1	1.79	0.81
1:B:107:ASP:OD1	7:B:2054:HOH:O	1.98	0.80
1:B:164:PHE:HE2	1:B:166:THR:CG2	2.08	0.66
2:A:1259:NGA:H83	2:A:1261:SIA:H92	1.76	0.66
1:B:233:ILE:N	1:B:233:ILE:HD12	2.12	0.65
1:B:164:PHE:HE2	1:B:166:THR:HG22	1.62	0.65
4:A:1263:MPD:H12	4:A:1263:MPD:H52	1.71	0.63
1:A:14:LYS:NZ	1:B:69:GLN:OE1	2.26	0.63
1:B:177:ASN:C	1:B:177:ASN:OD1	2.35	0.62
1:A:2:LYS:CG	1:A:3:LYS:H	1.98	0.62
1:A:18:TYR:CE2	1:A:233:ILE:HD11	2.34	0.62
1:B:166:THR:HG21	7:B:2008:HOH:O	1.98	0.61
4:A:1263:MPD:C4	7:A:2078:HOH:O	2.31	0.61
1:A:157:GLN:HG3	7:A:2104:HOH:O	2.02	0.59
1:B:90:ASN:OD1	7:B:2039:HOH:O	2.16	0.58
1:B:164:PHE:CE2	1:B:166:THR:CG2	2.86	0.57
1:A:14:LYS:HE3	1:A:163:ALA:O	2.05	0.57
5:B:1262:CH:H5''	5:B:1262:CH:H6	1.85	0.56
1:A:230:ASN:ND2	7:A:2135:HOH:O	2.38	0.54
1:A:87:GLU:CG	7:A:2057:HOH:O	2.56	0.53
1:A:177:ASN:H	1:A:177:ASN:ND2	2.06	0.53
1:B:164:PHE:CE2	1:B:166:THR:HG22	2.45	0.52
1:A:87:GLU:HG3	7:A:2057:HOH:O	2.08	0.52
1:A:93:LYS:NZ	7:A:2065:HOH:O	2.32	0.52
2:A:1259:NGA:H83	2:A:1261:SIA:C9	2.39	0.52
1:B:32:GLN:HE21	1:B:58:GLN:HE22	1.57	0.52
1:B:2:LYS:CG	1:B:3:LYS:N	2.51	0.51
5:B:1262:CH:C6	5:B:1262:CH:C5'	2.73	0.49
1:A:156:TYR:O	1:A:157:GLN:HB2	2.12	0.49
4:A:1263:MPD:H32	7:A:2078:HOH:O	2.14	0.48
1:A:228:ASN:OD1	7:A:2134:HOH:O	2.20	0.47
1:A:45:CYS:O	1:A:73:THR:HA	2.15	0.47
1:B:233:ILE:H	1:B:233:ILE:HD12	1.80	0.46
1:B:206:ILE:HD12	1:B:206:ILE:C	2.36	0.46
1:A:67:GLN:NE2	7:A:2042:HOH:O	2.47	0.45
1:A:206:ILE:HD12	1:A:206:ILE:C	2.39	0.43
1:B:233:ILE:CD1	1:B:233:ILE:N	2.81	0.42
4:A:1263:MPD:O2	4:A:1263:MPD:H52	2.19	0.42
1:B:190:LYS:O	1:B:194:ILE:HG13	2.20	0.41
1:B:93:LYS:HD3	7:B:2039:HOH:O	2.21	0.41

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	241/258 (93%)	239 (99%)	2 (1%)	0	100	100
1	B	237/258 (92%)	233 (98%)	4 (2%)	0	100	100
All	All	478/516 (93%)	472 (99%)	6 (1%)	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	224/233 (96%)	223 (100%)	1 (0%)	93	93
1	B	220/233 (94%)	217 (99%)	3 (1%)	74	70
All	All	444/466 (95%)	440 (99%)	4 (1%)	84	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	B	111	GLN
1	B	216	LEU
1	B	235	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	83	GLN
1	A	157	GLN
1	A	177	ASN
1	A	214	ASN
1	A	228	ASN
1	A	230	ASN
1	B	9	ASN
1	B	32	GLN
1	B	191	ASN
1	B	214	ASN
1	B	219	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	$\# Z  > 2$
2	NGA	A	1259	2	15,15,15	1.39	1 (6%)	17,21,21	1.15	2 (11%)
2	GAL	A	1260	2	9,10,12	0.79	0	10,13,17	0.73	0
2	SIA	A	1261	2	17,21,21	1.34	2 (11%)	19,31,31	1.89	4 (21%)
2	NGA	B	1259	2	15,15,15	1.31	1 (6%)	17,21,21	1.20	3 (17%)
2	GAL	B	1260	2	9,10,12	0.67	0	10,13,17	1.73	2 (20%)
2	SIA	B	1261	2	17,21,21	1.99	3 (17%)	19,31,31	1.62	3 (15%)

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	NGA	A	1259	2	-	0/6/26/26	0/1/1/1
2	GAL	A	1260	2	-	0/2/15/22	0/1/1/1
2	SIA	A	1261	2	1/1/8/9	0/14/38/38	0/1/1/1
2	NGA	B	1259	2	-	0/6/26/26	0/1/1/1
2	GAL	B	1260	2	-	0/2/15/22	0/1/1/1
2	SIA	B	1261	2	1/1/8/9	0/14/38/38	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1259	NGA	O6-C6	-4.36	1.23	1.42
2	A	1259	NGA	O6-C6	-4.34	1.23	1.42
2	A	1261	SIA	C3-C2	3.29	1.56	1.51
2	B	1261	SIA	C3-C2	3.34	1.56	1.51
2	A	1261	SIA	O2-C2	3.58	1.43	1.40
2	B	1261	SIA	O6-C2	4.45	1.47	1.42
2	B	1261	SIA	O2-C2	5.17	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1261	SIA	C7-C6-C5	-4.82	107.03	114.32
2	B	1260	GAL	C4-C3-C2	-4.16	105.56	111.55
2	B	1261	SIA	C7-C6-C5	-3.70	108.73	114.32
2	A	1261	SIA	O2-C2-C3	-3.14	105.49	109.41
2	B	1261	SIA	O2-C2-C3	-2.83	105.87	109.41
2	A	1259	NGA	C1-O5-C5	-2.39	109.04	113.47
2	B	1259	NGA	C6-C5-C4	-2.26	107.43	113.02
2	A	1261	SIA	O9-C9-C8	-2.20	106.31	111.10
2	B	1260	GAL	O5-C5-C6	-2.02	102.98	107.35
2	B	1259	NGA	O5-C5-C4	2.00	113.44	109.68
2	B	1259	NGA	O6-C6-C5	2.71	120.28	111.33
2	A	1259	NGA	O6-C6-C5	2.80	120.58	111.33
2	A	1261	SIA	O6-C6-C7	3.69	112.84	107.26
2	B	1261	SIA	O6-C6-C7	4.17	113.57	107.26

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1261	SIA	C8
2	A	1261	SIA	C8

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1259	NGA	2	0
2	A	1261	SIA	2	0

## 5.6 Ligand geometry [i](#)

8 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	ACT	A	1262	-	1,3,3	1.12	0	0,3,3	0.00	-
4	MPD	A	1263	-	6,7,7	0.38	0	7,10,10	0.48	0
5	CH	A	1264	-	17,22,22	1.76	4 (23%)	22,33,33	1.29	2 (9%)
3	ACT	A	1265	-	1,3,3	1.04	0	0,3,3	0.00	-
6	EDO	A	1266	-	3,3,3	0.49	0	2,2,2	0.36	0
5	CH	B	1262	-	17,22,22	1.83	4 (23%)	22,33,33	1.80	6 (27%)
6	EDO	B	1263	-	3,3,3	0.46	0	2,2,2	0.45	0
3	ACT	B	1264	-	1,3,3	1.25	0	0,3,3	0.00	-

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	ACT	A	1262	-	-	0/0/0/0	0/0/0/0
4	MPD	A	1263	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CH	A	1264	-	-	0/6/26/26	0/2/2/2
3	ACT	A	1265	-	-	0/0/0/0	0/0/0/0
6	EDO	A	1266	-	-	0/1/1/1	0/0/0/0
5	CH	B	1262	-	-	0/6/26/26	0/2/2/2
6	EDO	B	1263	-	-	0/1/1/1	0/0/0/0
3	ACT	B	1264	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1262	CH	O5'-C5'	-2.31	1.35	1.44
5	A	1264	CH	P-OP3	2.17	1.62	1.54
5	A	1264	CH	C4-N3	2.57	1.40	1.35
5	B	1262	CH	C4-N3	2.85	1.40	1.35
5	A	1264	CH	C6-N1	3.13	1.40	1.35
5	B	1262	CH	C6-N1	4.09	1.41	1.35
5	B	1262	CH	O4'-C1'	4.27	1.46	1.41
5	A	1264	CH	O4'-C1'	4.84	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1262	CH	O4'-C4'-C5'	-4.71	92.49	109.32
5	B	1262	CH	C5'-C4'-C3'	-3.19	102.53	115.21
5	A	1264	CH	C4'-O4'-C1'	-2.85	106.59	109.72
5	B	1262	CH	C4'-O4'-C1'	-2.73	106.71	109.72
5	B	1262	CH	O5'-P-OP1	2.05	112.36	107.14
5	B	1262	CH	OP2-P-O5'	2.15	112.75	106.56
5	B	1262	CH	C2-N3-C4	3.38	120.38	115.61
5	A	1264	CH	C2-N3-C4	3.86	121.06	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1263	MPD	9	0
5	B	1262	CH	5	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	245/258 (94%)	0.23	7 (2%) 55 65	21, 32, 49, 55	3 (1%)
1	B	243/258 (94%)	0.32	12 (4%) 33 45	24, 38, 62, 73	7 (2%)
All	All	488/516 (94%)	0.28	19 (3%) 43 54	21, 34, 56, 73	10 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ASN	3.6
1	B	237	ASN	3.3
1	B	238	ASN	3.1
1	A	24	ASP	3.0
1	B	258	ILE	2.8
1	B	255	SER	2.6
1	A	49	PHE	2.6
1	B	23	ASN	2.5
1	B	164	PHE	2.4
1	A	258	ILE	2.4
1	B	166	THR	2.4
1	B	157	GLN	2.4
1	A	78	CYS	2.3
1	B	191	ASN	2.2
1	A	30	CYS	2.2
1	A	189	SER	2.2
1	B	190	LYS	2.1
1	B	216	LEU	2.1
1	B	177	ASN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SIA	B	1261	21/21	0.89	0.14	0.70	39,42,47,51	0
2	SIA	A	1261	21/21	0.92	0.13	-1.13	27,32,37,44	0
2	NGA	B	1259	15/15	0.83	0.22	-	57,61,63,65	0
2	GAL	B	1260	10/12	0.84	0.17	-	50,53,55,56	0
2	GAL	A	1260	10/12	0.93	0.11	-	39,41,44,48	0
2	NGA	A	1259	15/15	0.87	0.22	-	45,49,55,58	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	B	1263	4/4	0.80	0.26	8.76	71,71,72,72	0
4	MPD	A	1263	8/8	0.85	0.25	7.51	45,48,51,51	0
5	CH	A	1264	21/21	0.97	0.14	0.28	25,28,29,29	0
5	CH	B	1262	21/21	0.93	0.13	0.19	39,41,44,46	0
3	ACT	B	1264	4/4	0.90	0.10	-	66,66,66,66	0
3	ACT	A	1265	4/4	0.88	0.10	-	70,70,70,70	0
6	EDO	A	1266	4/4	0.82	0.12	-	66,67,67,67	0
3	ACT	A	1262	4/4	0.91	0.14	-	62,62,62,62	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.