



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3FBY  
Title : The crystal structure of the signature domain of cartilage oligomeric matrix protein.  
Authors : Tan, K.; Lawler, J.  
Deposited on : 2008-11-20  
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

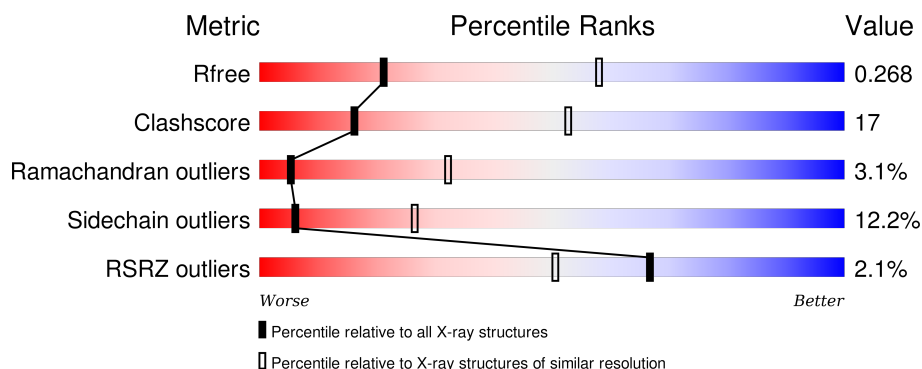
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	551	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	551	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>36%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	551	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>6%</div> <div>.</div> </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
3	MAN	A	903	X	-	-	-
4	SO4	A	1003	-	-	-	X
4	SO4	C	1003	-	-	-	X
5	NAG	B	901	X	-	-	-
5	MAN	B	903	X	-	-	-
6	MAN	C	903	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12777 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 Cartilage oligomeric matrix protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			
1	B	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			
1	C	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ARG	-	EXPRESSION TAG	UNP P49747
A	210	SER	-	EXPRESSION TAG	UNP P49747
A	211	PRO	-	EXPRESSION TAG	UNP P49747
A	212	TRP	-	EXPRESSION TAG	UNP P49747
A	213	PRO	-	EXPRESSION TAG	UNP P49747
A	214	GLY	-	EXPRESSION TAG	UNP P49747
A	215	VAL	-	EXPRESSION TAG	UNP P49747
A	216	PRO	-	EXPRESSION TAG	UNP P49747
A	217	THR	-	EXPRESSION TAG	UNP P49747
A	218	SER	-	EXPRESSION TAG	UNP P49747
A	219	PRO	-	EXPRESSION TAG	UNP P49747
A	220	VAL	-	EXPRESSION TAG	UNP P49747
A	221	TRP	-	EXPRESSION TAG	UNP P49747
A	222	TRP	-	EXPRESSION TAG	UNP P49747
A	223	ASN	-	EXPRESSION TAG	UNP P49747
A	224	SER	-	EXPRESSION TAG	UNP P49747
A	758	GLY	-	EXPRESSION TAG	UNP P49747
A	759	THR	-	EXPRESSION TAG	UNP P49747
B	209	ARG	-	EXPRESSION TAG	UNP P49747
B	210	SER	-	EXPRESSION TAG	UNP P49747
B	211	PRO	-	EXPRESSION TAG	UNP P49747
B	212	TRP	-	EXPRESSION TAG	UNP P49747
B	213	PRO	-	EXPRESSION TAG	UNP P49747

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Chain	Residue	Modelled	Actual	Comment	Reference
B	214	GLY	-	EXPRESSION TAG	UNP P49747
B	215	VAL	-	EXPRESSION TAG	UNP P49747
B	216	PRO	-	EXPRESSION TAG	UNP P49747
B	217	THR	-	EXPRESSION TAG	UNP P49747
B	218	SER	-	EXPRESSION TAG	UNP P49747
B	219	PRO	-	EXPRESSION TAG	UNP P49747
B	220	VAL	-	EXPRESSION TAG	UNP P49747
B	221	TRP	-	EXPRESSION TAG	UNP P49747
B	222	TRP	-	EXPRESSION TAG	UNP P49747
B	223	ASN	-	EXPRESSION TAG	UNP P49747
B	224	SER	-	EXPRESSION TAG	UNP P49747
B	758	GLY	-	EXPRESSION TAG	UNP P49747
B	759	THR	-	EXPRESSION TAG	UNP P49747
C	209	ARG	-	EXPRESSION TAG	UNP P49747
C	210	SER	-	EXPRESSION TAG	UNP P49747
C	211	PRO	-	EXPRESSION TAG	UNP P49747
C	212	TRP	-	EXPRESSION TAG	UNP P49747
C	213	PRO	-	EXPRESSION TAG	UNP P49747
C	214	GLY	-	EXPRESSION TAG	UNP P49747
C	215	VAL	-	EXPRESSION TAG	UNP P49747
C	216	PRO	-	EXPRESSION TAG	UNP P49747
C	217	THR	-	EXPRESSION TAG	UNP P49747
C	218	SER	-	EXPRESSION TAG	UNP P49747
C	219	PRO	-	EXPRESSION TAG	UNP P49747
C	220	VAL	-	EXPRESSION TAG	UNP P49747
C	221	TRP	-	EXPRESSION TAG	UNP P49747
C	222	TRP	-	EXPRESSION TAG	UNP P49747
C	223	ASN	-	EXPRESSION TAG	UNP P49747
C	224	SER	-	EXPRESSION TAG	UNP P49747
C	758	GLY	-	EXPRESSION TAG	UNP P49747
C	759	THR	-	EXPRESSION TAG	UNP P49747

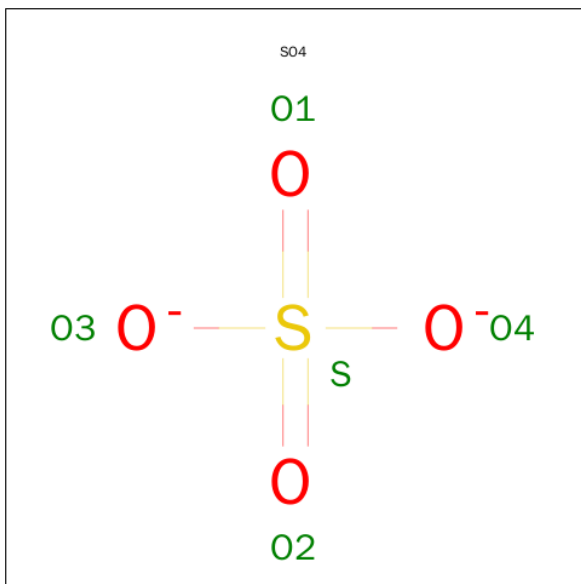
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	29	Total Ca 29 29	0	0
2	A	30	Total Ca 30 30	0	0
2	C	29	Total Ca 29 29	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

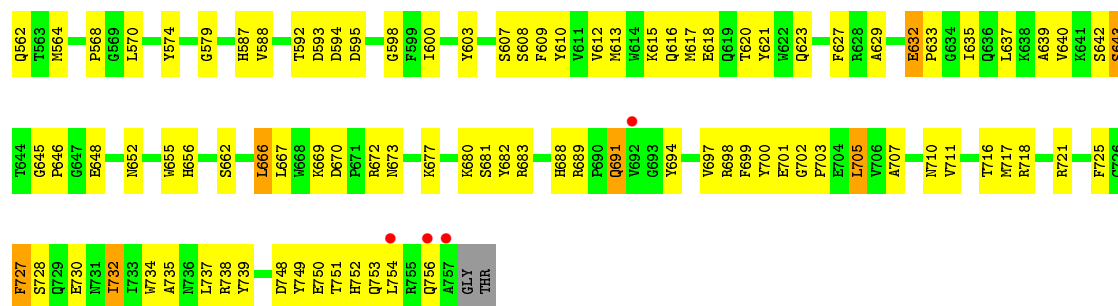
- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	5	Total	C	N	O	0	0
			61	34	2	25		

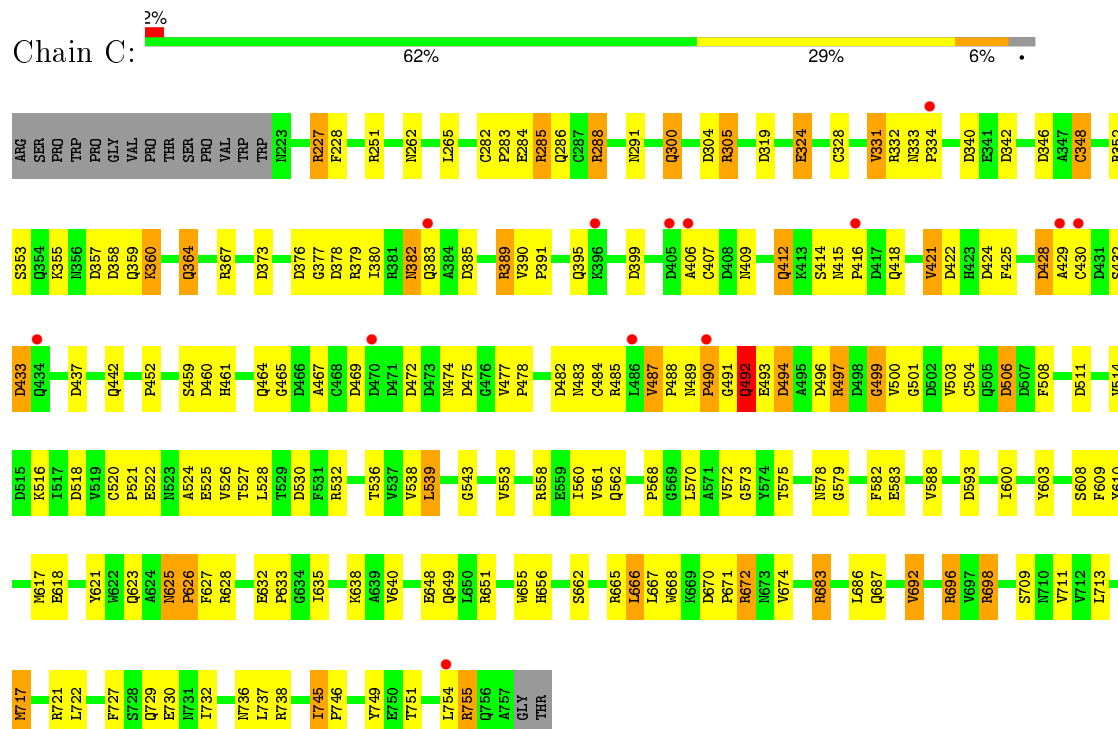
- Molecule 7 is water.

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





• Molecule 1: Cartilage oligomeric matrix protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.24Å 192.24Å 145.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 3.15 39.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.00-3.15) 99.7 (39.00-3.15)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, $R_{free}$	0.202 , 0.266 0.204 , 0.268	Depositor DCC
$R_{free}$ test set	2735 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 83.7	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53803 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: SO4, CA, NAG, MAN

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	0.72	1/4245 (0.0%)	0.82	0/5770
1	B	0.65	3/4245 (0.1%)	0.78	1/5770 (0.0%)
1	C	0.66	0/4245	0.79	1/5770 (0.0%)
All	All	0.68	4/12735 (0.0%)	0.80	2/17310 (0.0%)

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
3	A	1	0
5	B	2	0
6	C	1	0
All	All	4	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	CYS	CB-SG	-7.22	1.70	1.82
1	B	335	ASP	CB-CG	6.03	1.64	1.51
1	A	371	CYS	CB-SG	-5.96	1.72	1.81
1	B	371	CYS	CB-SG	-5.14	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	VAL	CB-CA-C	-5.33	101.27	111.40
1	C	754	LEU	CA-CB-CG	5.05	126.92	115.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	903	MAN	C1
5	B	901	NAG	C1
5	B	903	MAN	C1
6	C	903	MAN	C1

There are no planarity outliers.

## 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	4161	0	3698	124	0
1	B	4161	0	3698	160	0
1	C	4161	0	3698	120	0
2	A	30	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
3	A	50	0	43	3	0
4	A	25	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	1	0
5	B	39	0	34	0	0
6	C	61	0	52	0	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
All	All	12777	0	11223	403	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 17.

The worst 5 of 403 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:B:251:ARG:HH11	1:B:251:ARG:HG3	1.04	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:CYS:HB2	1:A:263:GLY:HA3	1.39	1.01
1:B:749:TYR:O	1:B:753:GLN:HG2	1.69	0.93
1:B:570:LEU:HD22	1:B:600:ILE:CD1	1.99	0.92
1:A:337:ARG:HH21	1:A:337:ARG:HG3	1.35	0.89

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	533/551 (97%)	443 (83%)	74 (14%)	16 (3%)	5	34
1	B	533/551 (97%)	435 (82%)	82 (15%)	16 (3%)	5	34
1	C	533/551 (97%)	443 (83%)	72 (14%)	18 (3%)	5	29
All	All	1599/1653 (97%)	1321 (83%)	228 (14%)	50 (3%)	5	32

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	B	474	ASN
1	B	543	GLY
1	C	352	ARG
1	C	379	ARG

### 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	459/473 (97%)	394 (86%)	65 (14%)	4	19
1	B	459/473 (97%)	410 (89%)	49 (11%)	8	32
1	C	459/473 (97%)	405 (88%)	54 (12%)	6	28
All	All	1377/1419 (97%)	1209 (88%)	168 (12%)	6	26

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	413	LYS
1	B	588	VAL
1	C	672	ARG
1	B	450	THR
1	B	497	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	546	GLN
1	B	691	GLN
1	C	649	GLN
1	B	562	GLN
1	B	587	HIS

### 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
3	NAG	A	901	1,3	14,14,15	0.57	0	15,19,21	2.10	7 (46%)
3	NAG	A	902	3	14,14,15	0.74	0	15,19,21	1.36	2 (13%)
3	MAN	A	903	3	11,11,12	1.00	1 (9%)	14,15,17	1.29	1 (7%)
3	MAN	A	904	3	11,11,12	0.80	0	14,15,17	1.52	1 (7%)
5	NAG	B	901	1,5	14,14,15	0.85	0	15,19,21	1.23	2 (13%)
5	NAG	B	902	5	14,14,15	0.80	1 (7%)	15,19,21	1.83	4 (26%)
5	MAN	B	903	5	11,11,12	0.64	0	14,15,17	1.60	2 (14%)
6	NAG	C	901	1,6	14,14,15	0.60	0	15,19,21	1.07	1 (6%)
6	NAG	C	902	6	14,14,15	0.87	0	15,19,21	2.05	4 (26%)
6	MAN	C	903	6	11,11,12	0.58	0	14,15,17	1.55	3 (21%)
6	MAN	C	904	6	11,11,12	0.51	0	14,15,17	1.53	2 (14%)
6	MAN	C	905	6	11,11,12	0.81	0	14,15,17	1.96	5 (35%)

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	NAG	A	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	902	3	-	0/6/23/26	0/1/1/1
3	MAN	A	903	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	904	3	-	0/2/19/22	0/1/1/1
5	NAG	B	901	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	902	5	-	0/6/23/26	0/1/1/1
5	MAN	B	903	5	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	C	901	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	902	6	-	0/6/23/26	0/1/1/1
6	MAN	C	903	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	904	6	-	0/2/19/22	0/1/1/1
6	MAN	C	905	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	NAG	O5-C1	-2.16	1.40	1.43
3	A	903	MAN	C2-C3	2.19	1.55	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	902	NAG	C2-N2-C7	-5.38	116.13	123.04
5	B	902	NAG	C4-C3-C2	-3.56	105.69	111.23
6	C	902	NAG	C3-C2-N2	-3.52	102.12	110.56
6	C	902	NAG	O4-C4-C3	-2.96	103.67	110.34
3	A	902	NAG	O4-C4-C3	-2.95	103.70	110.34

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	903	MAN	C1
6	C	903	MAN	C1
3	A	903	MAN	C1
5	B	901	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	NAG	2	0
3	A	902	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 88 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	1001	-	4,4,4	0.21	0	6,6,6	0.37	0
4	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.35	0
4	SO4	A	1003	-	4,4,4	0.23	0	6,6,6	0.12	0
4	SO4	A	1004	-	4,4,4	0.07	0	6,6,6	0.18	0
4	SO4	A	1005	-	4,4,4	0.18	0	6,6,6	0.10	0
4	SO4	B	1001	-	4,4,4	0.16	0	6,6,6	0.31	0
4	SO4	B	1002	-	4,4,4	0.26	0	6,6,6	0.43	0
4	SO4	C	1001	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	C	1002	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	C	1003	-	4,4,4	0.27	0	6,6,6	0.22	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
4	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1003	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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
4	C	1003	SO4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	535/551 (97%)	-0.09	9 (1%) 73 59	33, 49, 76, 91	0
1	B	535/551 (97%)	0.03	11 (2%) 67 50	24, 54, 70, 82	0
1	C	535/551 (97%)	0.01	13 (2%) 62 45	38, 54, 77, 85	0
All	All	1605/1653 (97%)	-0.02	33 (2%) 67 50	24, 52, 75, 91	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	754	LEU	4.9
1	C	429	ALA	4.0
1	B	757	ALA	3.5
1	A	495	ALA	3.1
1	C	406	ALA	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
5	NAG	B	901	14/15	0.94	0.15	-1.27	78,84,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	901	14/15	0.95	0.14	-1.41	61,67,71,74	0
6	NAG	C	901	14/15	0.96	0.17	-1.87	64,69,72,77	0
6	MAN	C	904	11/12	0.73	0.27	-	84,88,90,90	11
6	MAN	C	905	11/12	0.72	0.40	-	87,91,93,95	11
5	NAG	B	902	14/15	0.91	0.21	-	84,86,90,93	14
5	MAN	B	903	11/12	0.80	0.23	-	85,89,90,90	11
6	MAN	C	903	11/12	0.87	0.19	-	91,93,95,95	11
3	MAN	A	903	11/12	0.89	0.23	-	96,98,101,101	11
6	NAG	C	902	14/15	0.91	0.18	-	79,82,85,90	0
3	NAG	A	902	14/15	0.91	0.19	-	70,81,90,91	0
3	MAN	A	904	11/12	0.86	0.24	-	97,99,100,100	11

## 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	1003	5/5	0.75	0.39	4.89	106,107,107,107	5
4	SO4	C	1003	5/5	0.80	0.37	3.03	97,97,98,98	5
4	SO4	A	1002	5/5	0.87	0.27	1.56	94,94,97,97	5
2	CA	B	828	1/1	0.92	0.20	0.81	69,69,69,69	0
2	CA	C	828	1/1	0.97	0.20	0.78	58,58,58,58	0
2	CA	C	810	1/1	0.85	0.27	0.38	174,174,174,174	0
2	CA	C	801	1/1	0.97	0.20	0.01	52,52,52,52	0
2	CA	A	802	1/1	1.00	0.16	-0.03	58,58,58,58	0
2	CA	B	829	1/1	0.83	0.17	-0.14	89,89,89,89	0
2	CA	B	804	1/1	0.94	0.16	-0.17	83,83,83,83	0
2	CA	A	826	1/1	0.99	0.15	-0.41	86,86,86,86	0
2	CA	C	802	1/1	0.99	0.17	-0.52	50,50,50,50	0
2	CA	B	825	1/1	0.98	0.15	-0.55	111,111,111,111	0
2	CA	A	807	1/1	0.96	0.15	-0.57	61,61,61,61	0
2	CA	B	801	1/1	0.96	0.18	-0.61	70,70,70,70	0
2	CA	A	801	1/1	0.99	0.15	-0.65	56,56,56,56	0
2	CA	B	826	1/1	0.96	0.14	-0.68	86,86,86,86	0
2	CA	B	827	1/1	0.99	0.14	-0.78	62,62,62,62	0
2	CA	B	807	1/1	0.98	0.15	-0.81	56,56,56,56	0
2	CA	C	817	1/1	0.97	0.14	-0.81	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	C	807	1/1	0.96	0.13	-0.83	65,65,65,65	0
2	CA	A	821	1/1	0.81	0.16	-0.83	104,104,104,104	0
2	CA	B	820	1/1	0.96	0.14	-0.86	118,118,118,118	0
2	CA	B	803	1/1	0.97	0.14	-0.88	65,65,65,65	0
2	CA	A	817	1/1	0.99	0.14	-0.96	81,81,81,81	0
2	CA	A	803	1/1	0.96	0.13	-0.96	76,76,76,76	0
2	CA	B	805	1/1	0.99	0.14	-1.04	55,55,55,55	0
2	CA	A	828	1/1	0.96	0.14	-1.04	54,54,54,54	0
2	CA	B	818	1/1	0.98	0.13	-1.08	106,106,106,106	0
2	CA	B	806	1/1	0.99	0.12	-1.12	54,54,54,54	0
2	CA	C	827	1/1	0.98	0.13	-1.12	47,47,47,47	0
2	CA	A	812	1/1	0.97	0.09	-1.17	70,70,70,70	0
2	CA	B	810	1/1	0.92	0.07	-1.23	109,109,109,109	0
2	CA	C	805	1/1	0.97	0.13	-1.28	75,75,75,75	0
2	CA	A	811	1/1	0.94	0.11	-1.29	75,75,75,75	0
2	CA	A	827	1/1	0.98	0.14	-1.30	64,64,64,64	0
2	CA	A	800	1/1	0.86	0.16	-1.31	65,65,65,65	0
2	CA	A	805	1/1	0.94	0.12	-1.34	60,60,60,60	0
2	CA	C	806	1/1	0.98	0.09	-1.40	72,72,72,72	0
2	CA	B	817	1/1	0.98	0.09	-1.40	127,127,127,127	0
2	CA	A	806	1/1	0.99	0.10	-1.41	54,54,54,54	0
2	CA	C	809	1/1	0.84	0.09	-1.44	108,108,108,108	0
2	CA	C	821	1/1	0.65	0.12	-1.51	95,95,95,95	0
2	CA	B	815	1/1	0.98	0.07	-1.54	103,103,103,103	0
2	CA	A	818	1/1	0.98	0.09	-1.59	85,85,85,85	0
2	CA	B	821	1/1	0.91	0.10	-1.59	125,125,125,125	0
2	CA	A	823	1/1	0.94	0.07	-1.60	103,103,103,103	0
2	CA	A	825	1/1	0.95	0.11	-1.61	93,93,93,93	0
2	CA	C	820	1/1	0.91	0.06	-1.62	125,125,125,125	0
2	CA	C	812	1/1	0.91	0.11	-1.62	117,117,117,117	0
2	CA	C	811	1/1	0.96	0.10	-1.65	117,117,117,117	0
2	CA	B	808	1/1	0.99	0.11	-1.65	56,56,56,56	0
2	CA	A	822	1/1	0.91	0.09	-1.66	107,107,107,107	0
2	CA	B	823	1/1	0.85	0.09	-1.67	131,131,131,131	0
2	CA	B	811	1/1	0.86	0.07	-1.70	123,123,123,123	0
2	CA	C	825	1/1	0.92	0.08	-1.70	85,85,85,85	0
2	CA	A	820	1/1	0.95	0.06	-1.73	119,119,119,119	0
2	CA	A	808	1/1	0.99	0.09	-1.76	56,56,56,56	0
2	CA	B	819	1/1	0.96	0.08	-1.80	114,114,114,114	0
2	CA	C	803	1/1	0.98	0.10	-1.80	71,71,71,71	0
2	CA	A	819	1/1	0.97	0.07	-1.80	119,119,119,119	0
2	CA	C	808	1/1	0.97	0.09	-1.83	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	810	1/1	0.97	0.07	-1.84	104,104,104,104	0
2	CA	B	809	1/1	0.93	0.07	-1.85	85,85,85,85	0
2	CA	C	818	1/1	0.97	0.12	-1.86	94,94,94,94	0
2	CA	C	826	1/1	0.96	0.10	-1.87	85,85,85,85	0
2	CA	B	812	1/1	0.97	0.04	-1.87	87,87,87,87	0
2	CA	A	824	1/1	0.66	0.08	-1.90	160,160,160,160	0
2	CA	A	804	1/1	0.96	0.07	-1.92	78,78,78,78	0
2	CA	A	809	1/1	0.96	0.08	-1.93	65,65,65,65	0
2	CA	B	824	1/1	0.90	0.06	-2.03	140,140,140,140	0
2	CA	B	822	1/1	0.94	0.09	-2.06	114,114,114,114	0
2	CA	C	823	1/1	0.98	0.04	-2.07	111,111,111,111	0
2	CA	A	813	1/1	0.98	0.06	-2.13	81,81,81,81	0
2	CA	C	819	1/1	0.86	0.04	-2.15	118,118,118,118	0
2	CA	B	802	1/1	0.99	0.14	-2.16	53,53,53,53	0
2	CA	A	829	1/1	0.96	0.12	-2.22	95,95,95,95	0
2	CA	B	813	1/1	0.95	0.08	-2.29	111,111,111,111	0
2	CA	C	814	1/1	0.85	0.05	-2.29	119,119,119,119	0
2	CA	C	822	1/1	0.98	0.05	-2.30	118,118,118,118	0
2	CA	A	815	1/1	0.95	0.05	-2.41	115,115,115,115	0
2	CA	C	813	1/1	0.96	0.05	-2.50	119,119,119,119	0
2	CA	A	814	1/1	0.99	0.04	-2.54	101,101,101,101	0
2	CA	C	824	1/1	0.96	0.04	-2.65	115,115,115,115	0
2	CA	B	814	1/1	0.92	0.05	-2.78	121,121,121,121	0
2	CA	C	829	1/1	0.95	0.09	-2.91	109,109,109,109	0
2	CA	C	815	1/1	0.72	0.07	-2.96	125,125,125,125	0
2	CA	C	804	1/1	0.93	0.06	-4.00	74,74,74,74	0
4	SO4	C	1002	5/5	0.82	0.79	-	96,96,97,97	5
4	SO4	B	1001	5/5	0.95	0.18	-	82,82,85,85	0
2	CA	B	816	1/1	0.88	0.15	-	111,111,111,111	0
4	SO4	C	1001	5/5	0.91	0.30	-	88,89,89,89	5
2	CA	C	816	1/1	0.95	0.12	-	123,123,123,123	0
4	SO4	A	1001	5/5	0.93	0.38	-	104,105,106,106	5
4	SO4	B	1002	5/5	0.88	0.66	-	94,94,95,97	5
4	SO4	A	1005	5/5	0.72	0.54	-	108,108,108,108	5
2	CA	A	816	1/1	0.90	0.18	-	114,114,114,114	0
4	SO4	A	1004	5/5	0.76	0.32	-	105,106,106,106	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.