



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 04:56 pm GMT

PDB ID : 5AOQ  
Title : Structural basis of neurohormone perception by the receptor tyrosine kinase Torso  
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Deposited on : 2015-09-11  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

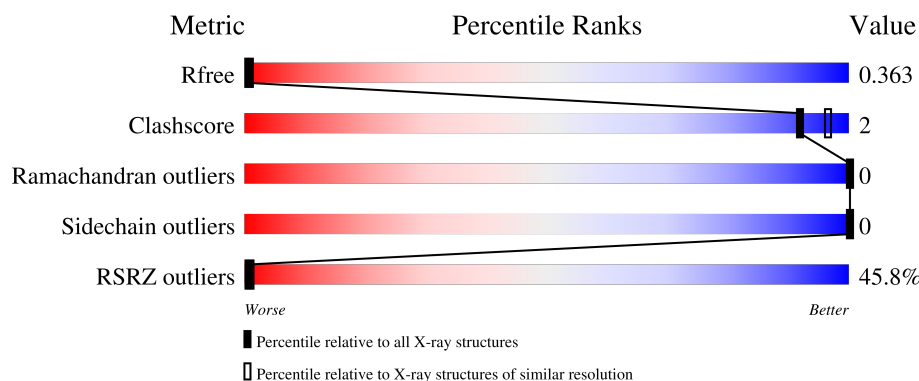
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	272	<div> <div>33%</div> <div>82%</div> <div>14%</div> </div>
1	B	272	<div> <div>30%</div> <div>82%</div> <div>14%</div> </div>
2	L	109	<div> <div>49%</div> <div>76%</div> <div>21%</div> </div>
2	M	109	<div> <div>62%</div> <div>74%</div> <div>6%</div> <div>19%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	2	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10381 atoms, of which 5076 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 TORSO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	233	Total	C	H	N	O	S	0	0	0
			3713	1228	1802	304	367	12			
1	B	233	Total	C	H	N	O	S	0	0	0
			3713	1228	1802	304	367	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP D2IYS2
A	-6	HIS	-	expression tag	UNP D2IYS2
A	-5	HIS	-	expression tag	UNP D2IYS2
A	-4	HIS	-	expression tag	UNP D2IYS2
A	-3	HIS	-	expression tag	UNP D2IYS2
A	-2	HIS	-	expression tag	UNP D2IYS2
A	-1	HIS	-	expression tag	UNP D2IYS2
A	0	HIS	-	expression tag	UNP D2IYS2
B	-7	HIS	-	expression tag	UNP D2IYS2
B	-6	HIS	-	expression tag	UNP D2IYS2
B	-5	HIS	-	expression tag	UNP D2IYS2
B	-4	HIS	-	expression tag	UNP D2IYS2
B	-3	HIS	-	expression tag	UNP D2IYS2
B	-2	HIS	-	expression tag	UNP D2IYS2
B	-1	HIS	-	expression tag	UNP D2IYS2
B	0	HIS	-	expression tag	UNP D2IYS2

- Molecule 2 is a protein called PREPROPTTH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	86	Total	C	H	N	O	S	0	0	0
			1396	439	695	122	133	7			
2	M	88	Total	C	H	N	O	S	0	2	0
			1449	455	723	127	137	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-4	SER	-	expression tag	UNP Q17238
L	-3	LEU	-	expression tag	UNP Q17238
L	-2	ASP	-	expression tag	UNP Q17238
L	36	GLN	ASN	engineered mutation	UNP Q17238
M	-4	SER	-	expression tag	UNP Q17238
M	-3	LEU	-	expression tag	UNP Q17238
M	-2	ASP	-	expression tag	UNP Q17238
M	36	GLN	ASN	engineered mutation	UNP Q17238

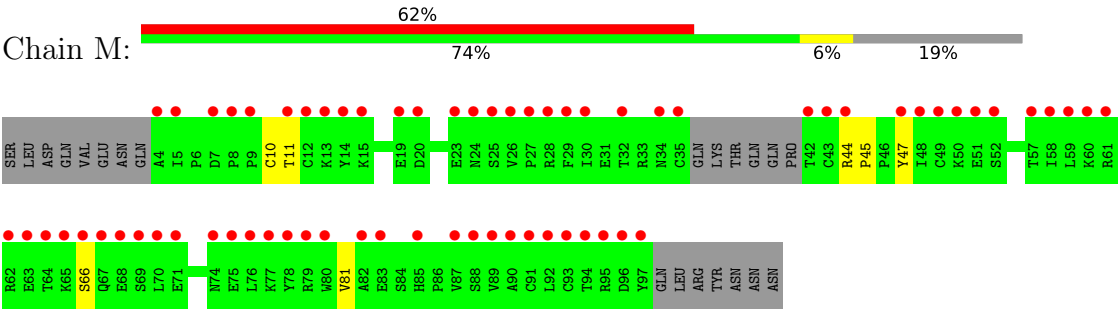
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
3	D	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			



● Molecule 2: PREPROPTTH



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.42Å 90.96Å 244.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.98-2.70) 97.2 (19.98-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 2.62Å)	Xtriage
Refinement program		Depositor
R, $R_{free}$	0.342 , 0.362 0.344 , 0.363	Depositor DCC
$R_{free}$ test set	1569 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	10381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8984e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG

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	0.23	0/1967	0.40	0/2682
1	B	0.22	0/1967	0.39	0/2682
2	L	0.23	0/715	0.47	0/964
2	M	0.23	0/757	0.41	0/1025
All	All	0.23	0/5406	0.41	0/7353

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	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	77	LYS	Peptide

### 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	1911	1802	1802	6	0
1	B	1911	1802	1802	5	0
2	L	701	695	692	1	0
2	M	726	723	710	4	0
3	C	28	27	25	2	0
3	D	28	27	25	1	0
All	All	5305	5076	5056	16	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 (16) 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:147:TYR:N	3:C:2:NAG:HO6	1.68	0.90
1:B:147:TYR:N	3:D:2:NAG:HO6	1.85	0.74
2:L:62:ARG:NH1	2:L:63:GLU:O	2.33	0.62
1:A:147:TYR:N	3:C:2:NAG:O6	2.33	0.61
1:A:174:THR:OG1	1:A:175:GLY:N	2.43	0.51
1:B:198:TRP:HB3	1:B:199:PRO:HD2	1.95	0.48
1:A:198:TRP:HB3	1:A:199:PRO:HD2	1.96	0.47
1:B:38:CYS:SG	1:B:40:THR:OG1	2.64	0.46
1:A:68:THR:HG21	1:A:77:PHE:CZ	2.53	0.43
1:A:81:GLU:CG	1:A:82:HIS:N	2.82	0.43
1:B:174:THR:OG1	1:B:175:GLY:N	2.52	0.42
2:M:10:CYS:SG	2:M:11:THR:N	2.92	0.42
2:M:45:PRO:HA	2:M:47:TYR:N	2.35	0.42
2:M:44:ARG:HB3	2:M:45:PRO:HD2	2.02	0.41
2:M:66:SER:HA	2:M:81:VAL:HG21	2.03	0.41
1:B:81:GLU:CG	1:B:82:HIS:N	2.84	0.41

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	229/272 (84%)	218 (95%)	11 (5%)	0	100	100
1	B	229/272 (84%)	218 (95%)	11 (5%)	0	100	100
2	L	82/109 (75%)	67 (82%)	15 (18%)	0	100	100
2	M	86/109 (79%)	75 (87%)	11 (13%)	0	100	100
All	All	626/762 (82%)	578 (92%)	48 (8%)	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	217/252 (86%)	217 (100%)	0	100	100
1	B	217/252 (86%)	217 (100%)	0	100	100
2	L	82/105 (78%)	82 (100%)	0	100	100
2	M	86/105 (82%)	86 (100%)	0	100	100
All	All	602/714 (84%)	602 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

4 monosaccharides 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	C	1	1,3	14,14,15	0.40	0	17,19,21	0.52	0
3	NAG	C	2	3	14,14,15	0.16	0	17,19,21	0.48	0
3	NAG	D	1	1,3	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.40	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	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

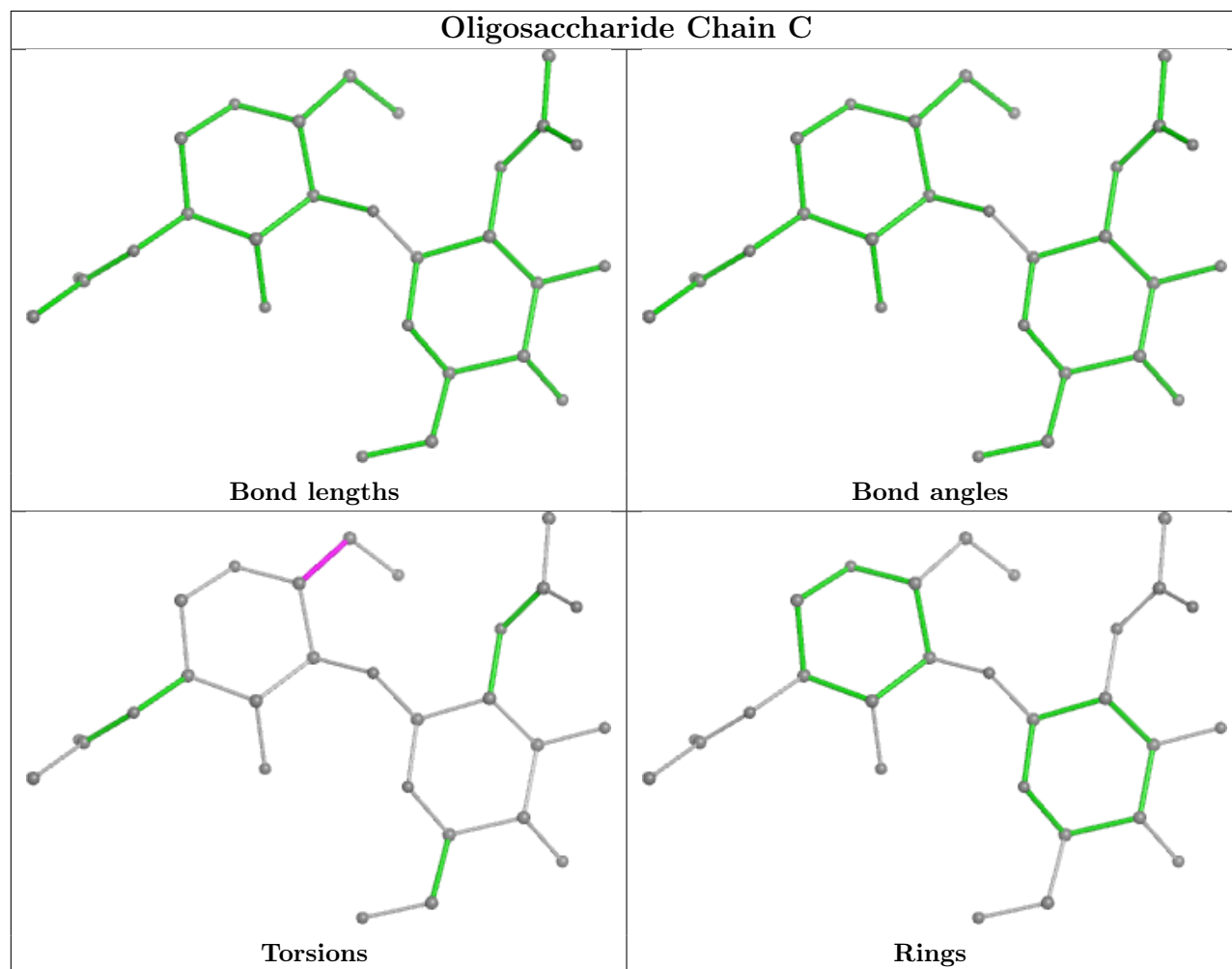
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

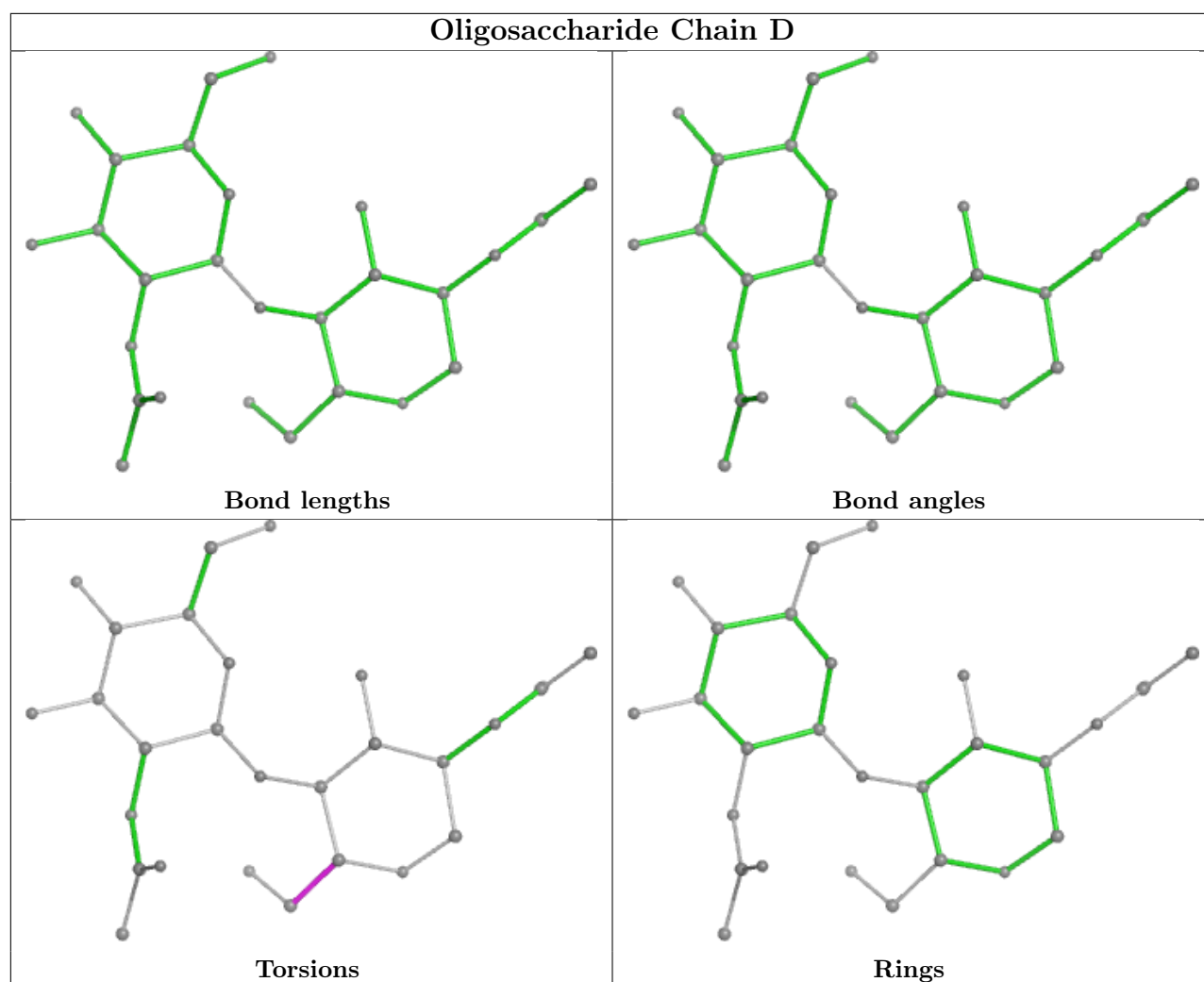
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	233/272 (85%)	1.98	90 (38%) <b>1</b> <b>1</b>	15, 51, 104, 178	0
1	B	233/272 (85%)	1.86	82 (35%) <b>1</b> <b>1</b>	6, 44, 90, 179	0
2	L	86/109 (78%)	3.18	53 (61%) <b>0</b> <b>1</b>	34, 76, 135, 170	0
2	M	88/109 (80%)	3.35	68 (77%) <b>0</b> <b>0</b>	32, 83, 132, 159	1 (1%)
All	All	640/762 (83%)	2.29	293 (45%) <b>1</b> <b>1</b>	6, 55, 124, 179	1 (0%)

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	TYR	12.8
1	B	178	ASP	12.1
2	L	10	CYS	9.5
2	L	43	CYS	9.3
2	L	78	TYR	9.2
1	B	179	LEU	9.2
2	L	62	ARG	9.1
1	A	151	GLN	8.3
2	M	62	ARG	8.3
2	L	75	GLU	8.3
2	L	67	GLN	8.0
1	B	163	TYR	8.0
1	A	179	LEU	8.0
2	M	94	THR	7.9
1	A	28	TYR	7.9
1	B	151	GLN	7.9
1	A	247	MET	7.7
2	M	66	SER	7.6
2	L	66	SER	7.3
1	A	178	ASP	7.3
2	M	63	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	160	ASN	7.2
2	L	64	THR	7.1
2	L	9	PRO	6.5
2	L	94	THR	6.4
1	B	149	VAL	6.3
1	A	106	ALA	6.3
1	B	176	ASP	6.3
2	M	43	CYS	6.3
1	A	175	GLY	6.1
1	A	177	ARG	6.0
2	M	50	LYS	5.9
1	A	152	GLU	5.9
1	B	175	GLY	5.8
1	B	180	CYS	5.8
2	M	24	ASN	5.8
2	M	47	TYR	5.8
2	L	36	GLN	5.7
1	A	164	THR	5.6
2	M	64	THR	5.6
2	L	63	GLU	5.6
2	L	60	LYS	5.6
2	M	67	GLN	5.6
1	A	180	CYS	5.4
2	M	97	TYR	5.4
2	L	76	LEU	5.4
2	M	52	SER	5.4
2	M	13	LYS	5.3
2	M	60	LYS	5.3
1	A	149	VAL	5.2
1	A	176	ASP	5.2
2	M	80[A]	TRP	5.2
1	B	177	ARG	5.2
2	L	26	VAL	5.2
1	A	33	THR	5.2
1	A	201	ALA	5.2
1	B	247	MET	5.1
2	L	73	PRO	5.0
2	L	11	THR	5.0
2	L	74	ASN	5.0
1	A	162	SER	4.9
1	A	249	PRO	4.9
2	L	79	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
2	M	4	ALA	4.9
1	A	29	TYR	4.9
1	B	29	TYR	4.8
1	B	25	SER	4.8
1	A	160	ASN	4.7
2	M	51	GLU	4.6
2	L	41	PRO	4.6
1	B	188	GLN	4.5
2	M	79[A]	ARG	4.5
2	M	29	PHE	4.5
1	A	37	ASP	4.4
1	B	162	SER	4.4
2	M	87	VAL	4.4
1	B	105	THR	4.4
1	A	191	ASN	4.4
2	M	26	VAL	4.3
2	M	61	ARG	4.3
2	M	65	LYS	4.2
2	M	12	CYS	4.2
2	M	9	PRO	4.2
2	M	70	LEU	4.2
2	L	69	SER	4.2
2	L	24	ASN	4.2
2	M	27	PRO	4.1
2	M	14	TYR	4.1
2	L	12	CYS	4.1
2	L	93	CYS	4.1
1	A	84	ASN	4.0
1	A	157	ILE	4.0
1	B	197	ILE	4.0
2	M	5	ILE	4.0
2	M	92	LEU	3.9
1	A	49	ASP	3.9
2	M	83	GLU	3.9
2	M	89	VAL	3.9
1	A	173	THR	3.8
2	L	72	ILE	3.8
1	B	119	GLU	3.8
2	M	23	GLU	3.8
2	L	89	VAL	3.7
2	M	25	SER	3.7
1	A	25	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	153	PHE	3.7
1	A	190	THR	3.7
1	B	165	ILE	3.7
2	L	65	LYS	3.7
2	L	92	LEU	3.7
2	M	48	ILE	3.7
1	B	85	PHE	3.7
1	B	62	ASN	3.6
1	B	174	THR	3.6
2	M	58	ILE	3.6
2	M	88	SER	3.6
1	A	197	ILE	3.6
1	B	28	TYR	3.6
2	L	47	TYR	3.6
2	L	81	VAL	3.6
2	L	58	ILE	3.6
1	A	159	GLY	3.6
1	B	164	THR	3.5
1	B	173	THR	3.5
2	L	46	PRO	3.5
2	L	80	TRP	3.5
2	M	28	ARG	3.5
1	B	221	LYS	3.5
1	B	103	ILE	3.4
1	B	107	ASN	3.4
2	L	48	ILE	3.4
2	M	49	CYS	3.4
1	A	115	THR	3.4
1	A	39	LYS	3.4
1	B	94	GLU	3.4
1	A	214	ASP	3.4
1	B	4	VAL	3.4
2	M	34	ASN	3.4
1	B	49	ASP	3.4
2	M	95	ARG	3.4
1	A	119	GLU	3.3
2	M	90	ALA	3.3
2	M	59	LEU	3.3
1	A	172	ASN	3.3
2	L	45	PRO	3.2
2	M	20	ASP	3.2
1	B	118	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	3.2
1	A	150	THR	3.1
1	A	118	ASP	3.1
2	M	7	ASP	3.1
1	A	64	ILE	3.1
1	B	202	HIS	3.1
2	M	8	PRO	3.1
2	M	91	CYS	3.1
1	B	246	ASN	3.0
1	A	198	TRP	3.0
1	B	249	PRO	3.0
1	A	24	TYR	3.0
2	L	18	ILE	3.0
2	L	91	CYS	3.0
1	A	189	ASN	3.0
1	B	106	ALA	3.0
1	B	34	SER	3.0
2	L	15	LYS	3.0
2	M	74	ASN	3.0
1	B	225	GLY	3.0
1	A	30	LEU	2.9
2	M	11	THR	2.9
1	A	120	TYR	2.9
1	A	61	LYS	2.9
2	L	77	LYS	2.9
1	B	120	TYR	2.9
1	A	26	LEU	2.9
1	B	104	THR	2.8
1	B	155	TYR	2.8
1	B	58	CYS	2.8
1	B	39	LYS	2.8
2	M	15	LYS	2.8
1	B	5	SER	2.8
1	B	115	THR	2.8
1	B	201	ALA	2.8
1	A	244	LEU	2.8
1	A	246	ASN	2.8
2	M	69	SER	2.8
1	A	70	PRO	2.8
1	A	165	ILE	2.8
1	B	84	ASN	2.8
1	B	72	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	147	TYR	2.8
2	L	71	GLU	2.7
1	B	61	LYS	2.7
2	M	78	TYR	2.7
1	B	219	HIS	2.7
2	L	44	ARG	2.7
2	M	44	ARG	2.7
2	M	85	HIS	2.7
1	A	161	ASP	2.7
1	A	218	ILE	2.7
1	A	174	THR	2.7
1	A	231	TYR	2.7
2	L	95	ARG	2.7
1	A	88	ILE	2.7
1	A	193	LYS	2.6
1	B	199	PRO	2.6
2	L	98	GLN	2.6
1	A	103	ILE	2.6
1	A	155	TYR	2.6
1	A	148	ASN	2.6
1	A	200	THR	2.6
2	M	68	GLU	2.6
1	B	189	ASN	2.6
1	B	157	ILE	2.6
2	M	35	CYS	2.6
1	A	87	PRO	2.6
2	L	42	THR	2.6
1	A	101	GLU	2.5
2	M	93	CYS	2.5
1	B	6	GLN	2.5
2	L	19	GLU	2.5
1	B	24	TYR	2.5
2	M	76	LEU	2.5
2	L	61	ARG	2.5
1	A	16	LYS	2.5
2	L	50	LYS	2.5
2	M	42	THR	2.5
2	M	82	ALA	2.5
1	B	158	LEU	2.5
1	A	188	GLN	2.5
1	B	152	GLU	2.4
1	B	159	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	M	57	THR	2.4
1	A	158	LEU	2.4
1	A	235	SER	2.4
1	A	4	VAL	2.4
1	A	44	GLU	2.4
1	A	10	PRO	2.4
1	A	69	GLU	2.4
1	A	248	GLU	2.4
1	A	219	HIS	2.4
1	A	27	TYR	2.4
2	L	97	TYR	2.4
1	A	133	LEU	2.3
2	M	77	LYS	2.3
1	B	124	GLN	2.3
1	B	27	TYR	2.3
1	B	205	PHE	2.3
2	M	30	ILE	2.3
1	B	37	ASP	2.3
1	B	204	SER	2.3
1	A	100	GLY	2.3
2	M	75	GLU	2.3
1	A	211	VAL	2.3
1	A	55	LYS	2.2
1	B	81	GLU	2.2
2	M	32	THR	2.2
1	A	223	ILE	2.2
2	L	82	ALA	2.2
1	A	104	THR	2.2
1	B	209	ASN	2.2
1	B	168	LYS	2.2
1	A	208	GLU	2.2
1	A	199	PRO	2.2
1	B	200	THR	2.2
1	A	147	TYR	2.2
1	A	194	HIS	2.2
1	B	74	TRP	2.2
1	A	97	ASN	2.2
2	M	96	ASP	2.2
1	B	22	VAL	2.2
2	M	71	GLU	2.1
1	A	53	THR	2.1
1	A	73	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	73	HIS	2.1
2	L	14	TYR	2.1
2	L	23	GLU	2.1
2	L	27	PRO	2.1
1	A	31	ASN	2.1
1	B	185	ASN	2.1
1	B	245	ASN	2.1
1	B	79	LEU	2.1
1	B	194	HIS	2.1
1	B	117	LEU	2.1
1	B	16	LYS	2.1
1	A	48	SER	2.1
1	A	245	ASN	2.1
1	B	30	LEU	2.1
2	M	19	GLU	2.0
1	A	205	PHE	2.0
2	L	68	GLU	2.0
1	A	192	MET	2.0
1	B	243	PHE	2.0
1	B	86	ASP	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](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.