



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 10:13 AM EDT

PDB ID : 4KPM  
Title : Crystal structure of the catalytic domain of RpfB from Mycobacterium tuberculosis in complex with triNAG  
Authors : Squeglia, F.; Ruggiero, A.; Berisio, R.  
Deposited on : 2013-05-14  
Resolution : 1.33 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

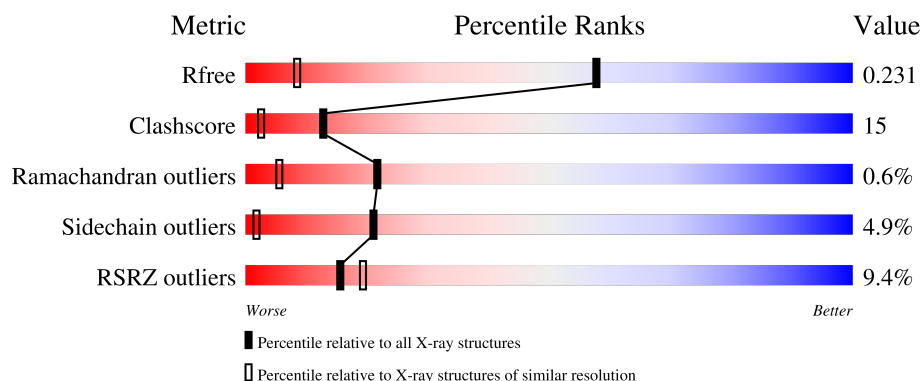
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.33 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	1904 (1.36-1.32)
Clashscore	180529	2038 (1.36-1.32)
Ramachandran outliers	177936	2016 (1.36-1.32)
Sidechain outliers	177891	2016 (1.36-1.32)
RSRZ outliers	164620	1903 (1.36-1.32)

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	80	<div> <div>8%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	B	80	<div> <div>9%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	80	<div> <div>12%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	D	80	<div> <div>9%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
2	E	3	<div> <div>100%</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
2	NAG	E	1	X	-	-	-

## 2 Entry composition

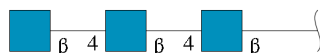
There are 5 unique types of molecules in this entry. The entry contains 3066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Resuscitation-promoting factor RpfB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			598	373	111	112	2			
1	B	80	Total	C	N	O	S	0	0	0
			598	373	111	112	2			
1	C	80	Total	C	N	O	S	0	0	0
			598	373	111	112	2			
1	D	80	Total	C	N	O	S	0	0	0
			598	373	111	112	2			

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



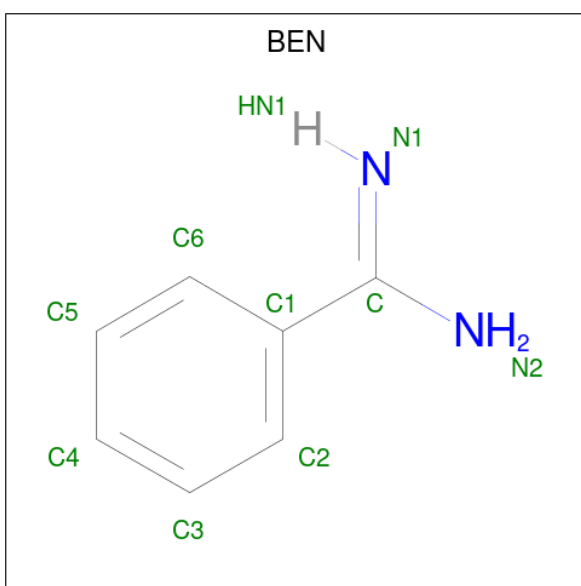
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is BENZAMIDINE (three-letter code: BEN) (formula:  $C_7H_8N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			9	7	2		

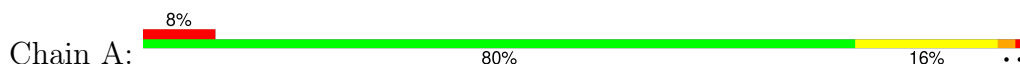
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total 166	O 166	0	0
5	B	162	Total 162	O 162	0	0
5	C	141	Total 141	O 141	0	0
5	D	144	Total 144	O 144	0	0

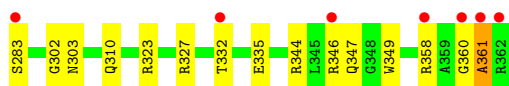
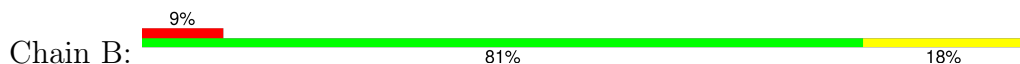
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

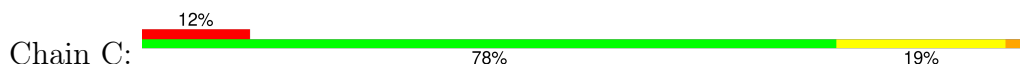
- Molecule 1: Resuscitation-promoting factor RpfB



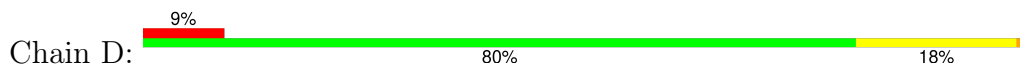
- Molecule 1: Resuscitation-promoting factor RpfB



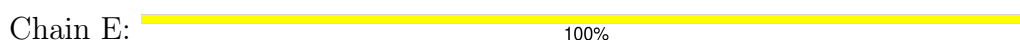
- Molecule 1: Resuscitation-promoting factor RpfB



- Molecule 1: Resuscitation-promoting factor RpfB



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.45Å 51.51Å 66.71Å 90.00° 104.39° 90.00°	Depositor
Resolution (Å)	15.00 – 1.33 15.00 – 1.33	Depositor EDS
% Data completeness (in resolution range)	83.3 (15.00-1.33) 83.3 (15.00-1.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.177 , 0.229 0.179 , 0.231	Depositor DCC
$R_{free}$ test set	2996 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, BEN

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	0.86	1/613 (0.2%)	0.90	0/835
1	B	0.85	0/613	0.91	2/835 (0.2%)
1	C	0.87	0/613	0.91	1/835 (0.1%)
1	D	0.82	0/613	1.08	5/835 (0.6%)
All	All	0.85	1/2452 (0.0%)	0.95	8/3340 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	ARG	CB-CG	5.03	1.66	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	ARG	NE-CZ-NH2	-13.58	113.51	120.30
1	D	344	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	B	327	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	D	345	LEU	CA-CB-CG	5.90	128.88	115.30
1	D	344	ARG	CD-NE-CZ	5.77	131.67	123.60
1	C	358	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	358	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	D	345	LEU	CB-CG-CD2	5.12	119.71	111.00

There are no chirality outliers.

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	598	0	549	12	0
1	B	598	0	549	16	0
1	C	598	0	549	26	2
1	D	598	0	549	17	1
2	E	42	0	37	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	B	9	0	7	0	0
5	A	166	0	0	2	0
5	B	162	0	0	3	2
5	C	141	0	0	7	0
5	D	144	0	0	5	1
All	All	3066	0	2240	70	3

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 15.

All (70) 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:C:344:ARG:HH21	1:C:345:LEU:CD2	1.63	1.11
1:C:344:ARG:HH21	1:C:345:LEU:HD23	0.95	1.07
1:A:283:SER:HA	5:A:4039:HOH:O	1.59	1.02
1:D:343:THR:HG23	1:D:347:GLN:HE22	1.18	1.01
1:C:344:ARG:NH2	1:C:345:LEU:HD23	1.78	0.97
1:D:343:THR:HG23	1:D:347:GLN:NE2	1.90	0.87
1:C:332:THR:HG21	5:C:618:HOH:O	1.77	0.83
1:C:283:SER:HB3	5:C:549:HOH:O	1.78	0.83
1:C:344:ARG:NH1	5:C:556:HOH:O	2.10	0.82
1:C:332:THR:HG23	1:C:335:GLU:H	1.45	0.81
1:D:332:THR:HG21	5:D:465:HOH:O	1.86	0.76
1:B:344:ARG:HD2	1:B:349:TRP:CZ2	2.21	0.76
1:D:332:THR:HG23	1:D:335:GLU:H	1.49	0.75
1:C:344:ARG:NH2	1:C:345:LEU:CD2	2.44	0.70
1:B:344:ARG:CD	1:B:349:TRP:CZ2	2.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:THR:CG2	1:D:347:GLN:NE2	2.57	0.67
1:D:362:ARG:O	1:D:362:ARG:HG3	1.94	0.66
1:B:332:THR:HG23	1:B:335:GLU:H	1.61	0.65
1:A:319:ASN:HD21	1:A:346:ARG:HH11	1.43	0.64
1:C:303:ASN:HD21	1:C:310:GLN:HE22	1.47	0.62
1:C:319:ASN:HA	5:C:623:HOH:O	1.98	0.62
1:D:343:THR:CG2	1:D:347:GLN:HE22	2.01	0.62
1:C:319:ASN:ND2	1:C:346:ARG:HD3	2.16	0.61
1:B:346:ARG:HB3	1:B:346:ARG:CZ	2.30	0.60
1:B:303:ASN:HD21	1:B:310:GLN:HE22	1.48	0.60
1:A:319:ASN:ND2	1:A:346:ARG:HH11	2.01	0.59
1:C:344:ARG:HD2	1:C:349:TRP:CZ2	2.38	0.58
1:A:303:ASN:HD21	1:A:310:GLN:HE22	1.49	0.58
1:C:332:THR:HB	5:C:537:HOH:O	2.05	0.56
1:A:319:ASN:HD22	1:A:342:VAL:HG12	1.71	0.55
1:A:349:TRP:HE1	1:A:362:ARG:HB2	1.70	0.55
1:C:332:THR:OG1	1:C:333:ARG:N	2.40	0.55
1:A:358:ARG:HD2	1:B:302:GLY:O	2.07	0.54
1:C:319:ASN:ND2	5:C:623:HOH:O	2.40	0.53
1:C:319:ASN:HD21	1:C:346:ARG:HD3	1.73	0.53
1:B:332:THR:HG22	1:B:335:GLU:CG	2.40	0.52
1:C:346:ARG:NH1	5:C:623:HOH:O	2.06	0.50
1:C:332:THR:HG22	1:C:335:GLU:CG	2.41	0.50
1:D:347:GLN:OE1	5:D:520:HOH:O	2.20	0.50
1:A:284:ILE:HD11	1:A:361:ALA:HB2	1.94	0.49
1:B:332:THR:HG22	1:B:335:GLU:HG3	1.94	0.49
1:D:303:ASN:HD21	1:D:310:GLN:HE22	1.60	0.49
1:D:332:THR:CG2	1:D:335:GLU:H	2.23	0.48
1:D:347:GLN:CD	5:D:520:HOH:O	2.51	0.47
1:C:344:ARG:HH21	1:C:345:LEU:HD21	1.70	0.47
1:A:323:ARG:HD3	5:A:4122:HOH:O	2.13	0.47
1:C:332:THR:HG22	1:C:335:GLU:HG3	1.96	0.47
1:B:344:ARG:HD2	1:B:349:TRP:HZ2	1.79	0.47
1:B:347:GLN:NE2	5:B:837:HOH:O	2.45	0.47
1:B:360:GLY:O	1:B:361:ALA:O	2.33	0.47
1:B:283:SER:HA	5:B:836:HOH:O	2.15	0.46
1:B:332:THR:CG2	1:B:335:GLU:H	2.27	0.46
1:D:347:GLN:NE2	5:D:456:HOH:O	2.49	0.46
1:B:360:GLY:HA2	5:B:950:HOH:O	2.16	0.45
1:C:332:THR:CG2	1:C:335:GLU:H	2.22	0.45
1:C:356:ALA:HB1	1:C:361:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:THR:HG22	1:D:335:GLU:CG	2.47	0.45
1:C:332:THR:CG2	1:C:335:GLU:HG3	2.47	0.44
1:B:344:ARG:HD3	1:B:349:TRP:CZ2	2.52	0.44
1:D:319:ASN:ND2	1:D:346:ARG:HH21	2.16	0.44
1:D:349:TRP:CD2	1:D:361:ALA:HB1	2.52	0.44
1:A:349:TRP:C	1:A:351:ALA:N	2.72	0.42
1:C:349:TRP:CD2	1:C:361:ALA:HB1	2.54	0.42
1:D:332:THR:OG1	1:D:333:ARG:N	2.52	0.42
1:B:303:ASN:HD21	1:B:310:GLN:NE2	2.16	0.41
1:A:344:ARG:HH21	1:A:362:ARG:CD	2.33	0.41
1:A:356:ALA:O	1:A:361:ALA:HB3	2.21	0.41
1:C:293:ALA:HB1	1:C:299:ILE:HG21	2.03	0.41
1:D:347:GLN:CG	5:D:520:HOH:O	2.68	0.41
1:C:344:ARG:NH2	1:C:345:LEU:HD21	2.31	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:GLY:O	1:D:360:GLY:O[2_546]	2.03	0.17
5:B:925:HOH:O	5:D:451:HOH:O[2_645]	2.16	0.04
1:C:323:ARG:NH2	5:B:881:HOH:O[1_455]	2.19	0.01

## 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	78/80 (98%)	76 (97%)	1 (1%)	1 (1%)	10	1
1	B	78/80 (98%)	75 (96%)	2 (3%)	1 (1%)	10	1
1	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
1	D	78/80 (98%)	76 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	312/320 (98%)	303 (97%)	7 (2%)	2 (1%)	22	5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	ALA
1	A	350	GLY

### 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	51/52 (98%)	48 (94%)	3 (6%)	16	1
1	B	51/52 (98%)	50 (98%)	1 (2%)	50	17
1	C	51/52 (98%)	48 (94%)	3 (6%)	16	1
1	D	51/52 (98%)	48 (94%)	3 (6%)	16	1
All	All	204/208 (98%)	194 (95%)	10 (5%)	21	2

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	A	344	ARG
1	A	358	ARG
1	B	323	ARG
1	C	283	SER
1	C	323	ARG
1	C	344	ARG
1	D	323	ARG
1	D	344	ARG
1	D	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	GLN
1	A	319	ASN
1	A	347	GLN
1	B	310	GLN
1	C	310	GLN
1	C	319	ASN
1	D	310	GLN
1	D	319	ASN
1	D	347	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

3 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	$\# Z  > 2$
2	NAG	E	1	2	14,14,15	0.71	0	17,19,21	1.56	3 (17%)
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	1.37	3 (17%)
2	NAG	E	3	2	14,14,15	0.52	0	17,19,21	1.27	3 (17%)

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	NAG	E	1	2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	3	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C5-C6	3.40	114.28	107.66
2	E	2	NAG	O4-C4-C3	-3.07	103.13	110.38
2	E	1	NAG	C4-C3-C2	2.67	114.94	111.02
2	E	3	NAG	O5-C5-C6	2.52	112.57	107.66
2	E	1	NAG	C3-C4-C5	2.28	114.36	110.23
2	E	3	NAG	O7-C7-C8	-2.26	118.03	122.05
2	E	2	NAG	O5-C1-C2	-2.17	107.94	111.29
2	E	2	NAG	O7-C7-N2	2.13	125.74	121.98
2	E	3	NAG	O7-C7-N2	2.13	125.74	121.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C5

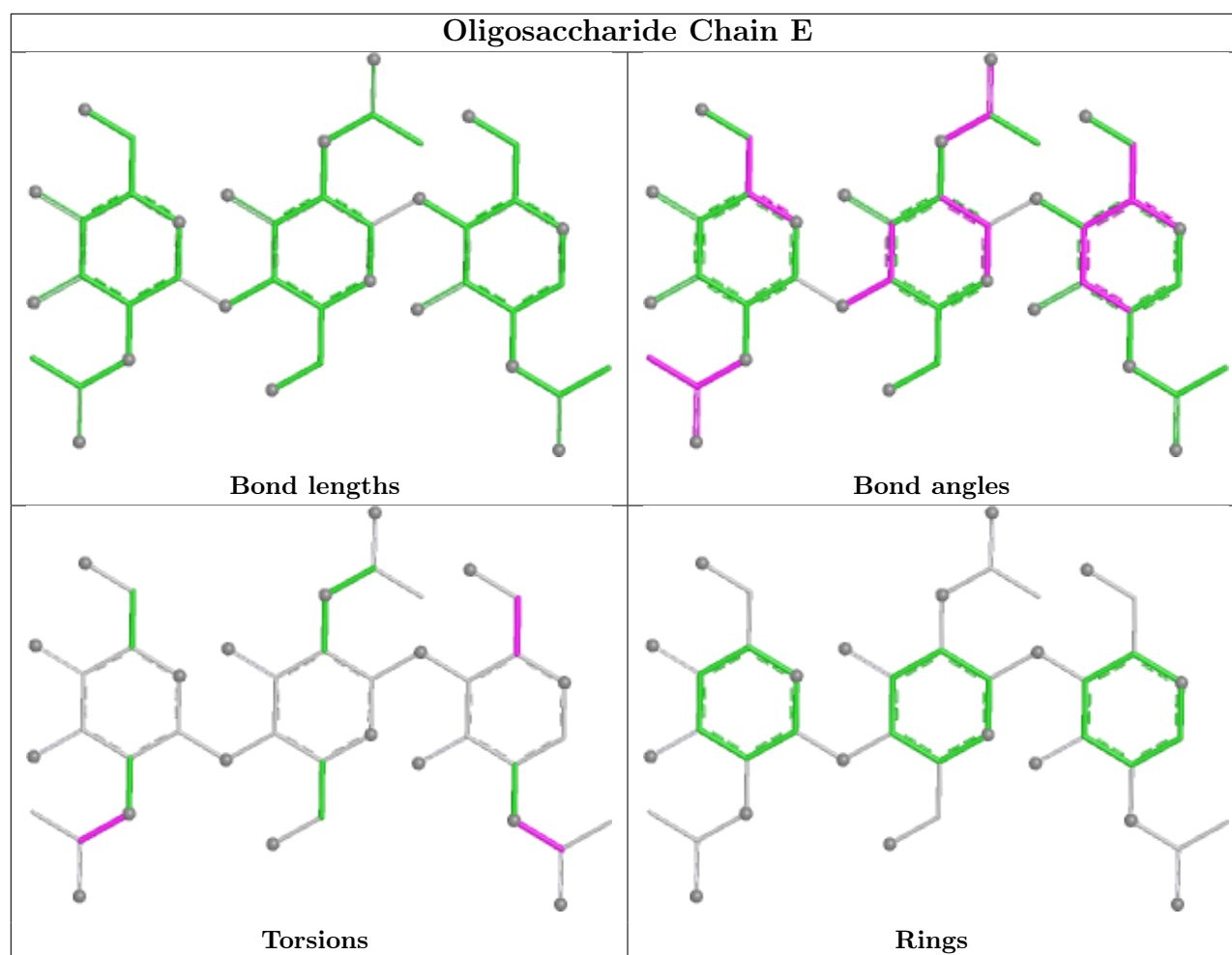
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	3	NAG	C8-C7-N2-C2
2	E	3	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

3 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	$\# Z  > 2$
4	BEN	B	701	-	9,9,9	1.51	1 (11%)	7,11,11	1.12	0
3	SO4	A	601	-	4,4,4	0.34	0	6,6,6	0.50	0
3	SO4	C	401	-	4,4,4	0.27	0	6,6,6	0.86	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	BEN	B	701	-	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	BEN	C1-C	-3.87	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	80/80 (100%)	0.57	6 (7%) 22 27	13, 16, 29, 43	0
1	B	80/80 (100%)	0.59	7 (8%) 17 21	12, 16, 29, 49	0
1	C	80/80 (100%)	0.55	10 (12%) 9 12	12, 16, 28, 44	0
1	D	80/80 (100%)	0.66	7 (8%) 17 21	14, 17, 31, 37	0
All	All	320/320 (100%)	0.59	30 (9%) 15 19	12, 16, 31, 49	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	ALA	6.8
1	B	361	ALA	6.2
1	B	360	GLY	5.6
1	D	360	GLY	4.9
1	B	283	SER	3.5
1	D	362	ARG	3.4
1	D	359	ALA	3.4
1	A	351	ALA	3.3
1	A	362	ARG	3.3
1	D	361	ALA	3.3
1	C	359	ALA	3.2
1	A	361	ALA	3.1
1	B	362	ARG	3.1
1	A	353	PRO	3.0
1	A	283	SER	2.8
1	C	362	ARG	2.7
1	D	283	SER	2.7
1	B	358	ARG	2.6
1	D	357	ALA	2.6
1	B	346	ARG	2.6
1	C	283	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	360	GLY	2.4
1	C	351	ALA	2.3
1	C	332	THR	2.2
1	A	345	LEU	2.2
1	C	350	GLY	2.1
1	D	332	THR	2.1
1	B	332	THR	2.1
1	C	344	ARG	2.0
1	C	349	TRP	2.0

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

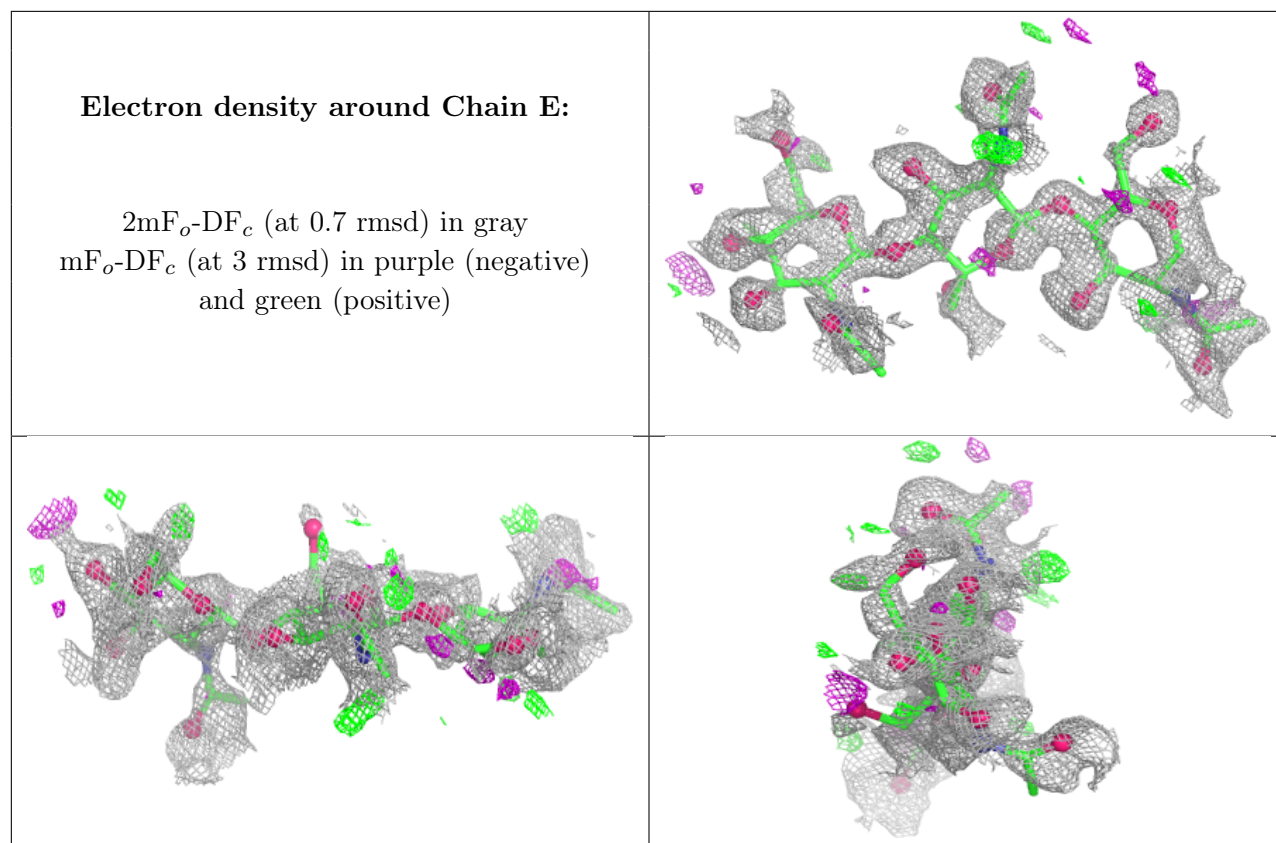
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	E	1	14/15	0.78	0.13	27,32,41,41	14
2	NAG	E	3	14/15	0.80	0.13	25,31,37,38	14
2	NAG	E	2	14/15	0.91	0.10	17,25,33,38	14

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BEN	B	701	9/9	0.90	0.09	20,22,24,25	0
3	SO4	C	401	5/5	0.95	0.07	20,24,27,28	0
3	SO4	A	601	5/5	0.97	0.05	17,17,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.