wwPDB X-ray Structure Validation Summary Report (i)

Feb 12, 2024 – 07:16 PM EST

PDB ID	:	3HST
Title	:	N-Terminal RNASE H domain of rv2228c from mycobacterium tuberculosis as a fusion protein with maltose binding protein
Authors	:	Watkins, H.A.; Baker, E.N.
Deposited on	:	2009-06-10
Resolution	:	2.25 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

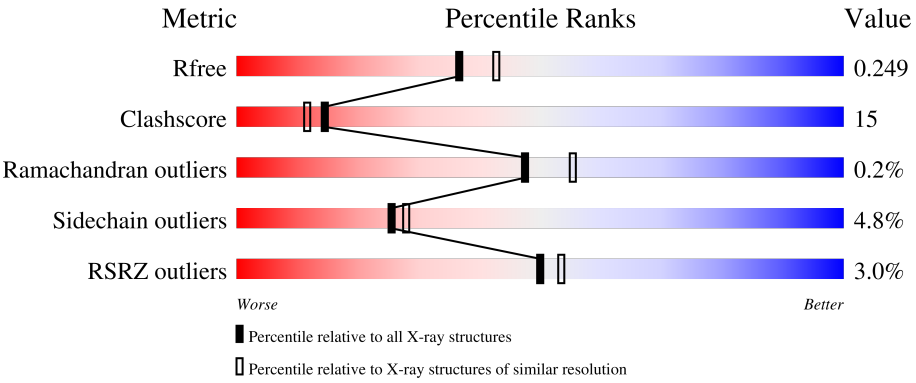
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 >=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 <=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	387	2% 77% 16% • 6%
1	C	387	2% 73% 20% • 5%
2	B	141	4% 59% 33% 6% ••
2	D	141	6% 66% 25% • 7%
3	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	3	33% 33% 33%

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
4	EDO	A	2	-	-	X	-
4	EDO	C	3	-	-	X	-
5	TAR	C	395	X	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8127 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2829	1820	460	543	6			
1	C	369	Total	C	N	O	S	0	0	0
			2859	1838	464	551	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP P0AEX9
A	375	ASN	-	expression tag	UNP P0AEX9
A	376	SER	-	expression tag	UNP P0AEX9
A	377	SER	-	expression tag	UNP P0AEX9
A	378	SER	-	expression tag	UNP P0AEX9
A	379	ASN	-	expression tag	UNP P0AEX9
A	380	ASN	-	expression tag	UNP P0AEX9
A	381	ASN	-	expression tag	UNP P0AEX9
A	382	ASN	-	expression tag	UNP P0AEX9
A	383	ASN	-	expression tag	UNP P0AEX9
A	384	ASN	-	expression tag	UNP P0AEX9
A	385	ASN	-	expression tag	UNP P0AEX9
A	386	ASN	-	expression tag	UNP P0AEX9
A	387	ASN	-	expression tag	UNP P0AEX9
A	388	ASN	-	expression tag	UNP P0AEX9
A	389	LEU	-	expression tag	UNP P0AEX9
A	390	GLY	-	expression tag	UNP P0AEX9
A	391	ILE	-	expression tag	UNP P0AEX9
A	392	GLU	-	expression tag	UNP P0AEX9
A	393	GLY	-	expression tag	UNP P0AEX9
A	394	ARG	-	expression tag	UNP P0AEX9
C	8	MET	-	expression tag	UNP P0AEX9
C	375	ASN	-	expression tag	UNP P0AEX9
C	376	SER	-	expression tag	UNP P0AEX9
C	377	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	SER	-	expression tag	UNP P0AEX9
C	379	ASN	-	expression tag	UNP P0AEX9
C	380	ASN	-	expression tag	UNP P0AEX9
C	381	ASN	-	expression tag	UNP P0AEX9
C	382	ASN	-	expression tag	UNP P0AEX9
C	383	ASN	-	expression tag	UNP P0AEX9
C	384	ASN	-	expression tag	UNP P0AEX9
C	385	ASN	-	expression tag	UNP P0AEX9
C	386	ASN	-	expression tag	UNP P0AEX9
C	387	ASN	-	expression tag	UNP P0AEX9
C	388	ASN	-	expression tag	UNP P0AEX9
C	389	LEU	-	expression tag	UNP P0AEX9
C	390	GLY	-	expression tag	UNP P0AEX9
C	391	ILE	-	expression tag	UNP P0AEX9
C	392	GLU	-	expression tag	UNP P0AEX9
C	393	GLY	-	expression tag	UNP P0AEX9
C	394	ARG	-	expression tag	UNP P0AEX9

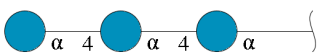
- Molecule 2 is a protein called Protein Rv2228c/MT2287.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1045	651	192	199	3			
2	D	131	Total	C	N	O	S	0	0	0
			999	625	183	188	3			

There are 4 discrepancies between the modelled and reference sequences:

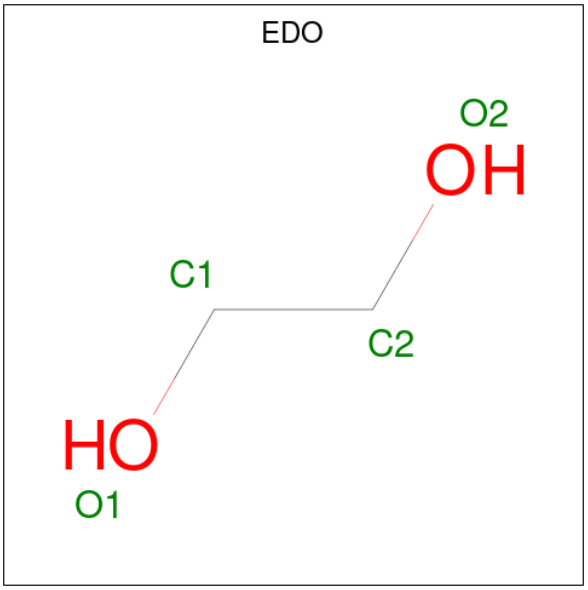
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P64955
B	1	VAL	-	expression tag	UNP P64955
D	0	SER	-	expression tag	UNP P64955
D	1	VAL	-	expression tag	UNP P64955

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



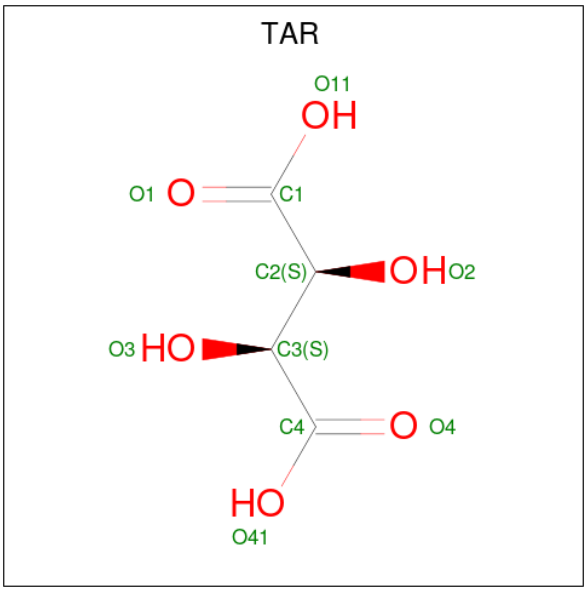
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	3	Total C O 34 18 16	0	0	0
3	F	3	Total C O 34 18 16	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 4 6	0	0

- Molecule 6 is water.

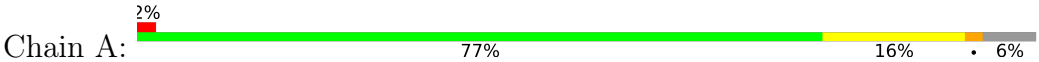
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	130	Total O 130 130	0	0
6	B	30	Total O 30 30	0	0
6	C	134	Total O 134 134	0	0
6	D	11	Total O 11 11	0	0

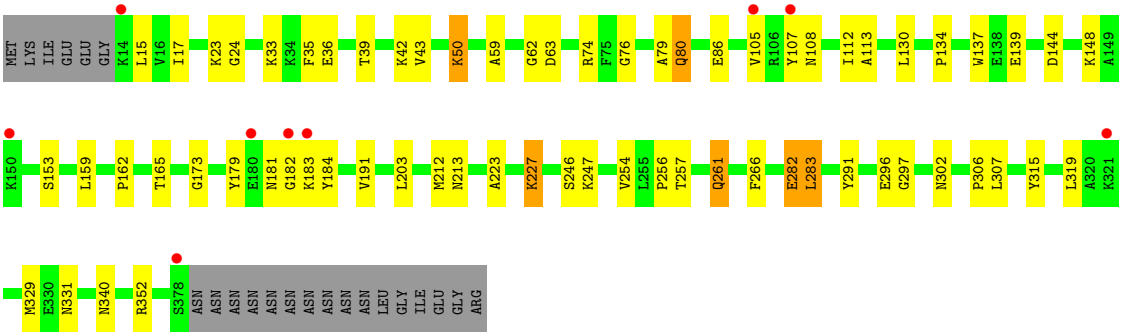
3 Residue-property plots (i)

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: Maltose-binding periplasmic protein

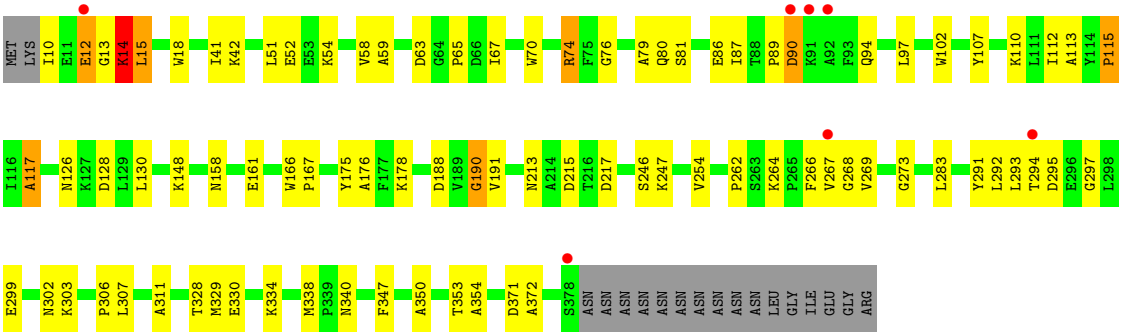
Chain A:





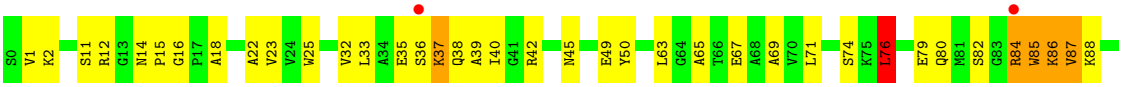
• Molecule 1: Maltose-binding periplasmic protein

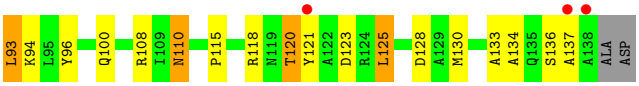
Chain C:



• Molecule 2: Protein Rv2228c/MT2287

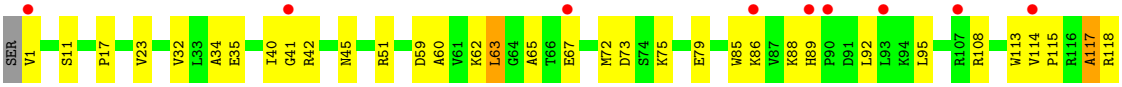
Chain B:

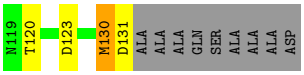




• Molecule 2: Protein Rv2228c/MT2287

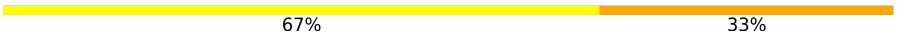
Chain D:





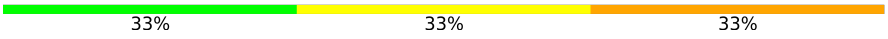
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.63Å 101.38Å 76.09Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	41.45 – 2.25 41.44 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.45-2.25) 100.0 (41.44-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0037, PHENIX	Depositor
R, R_{free}	0.183 , 0.239 0.210 , 0.249	Depositor DCC
R_{free} test set	2576 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8127	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GLC, EDO, TAR

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	1.02	1/2898 (0.0%)	0.88	5/3936 (0.1%)
1	C	1.09	1/2928 (0.0%)	0.92	7/3976 (0.2%)
2	B	1.00	0/1062	0.99	4/1441 (0.3%)
2	D	0.90	0/1016	0.85	3/1378 (0.2%)
All	All	1.03	2/7904 (0.0%)	0.91	19/10731 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLU	CB-CG	5.39	1.62	1.52
1	C	190	GLY	C-O	-5.01	1.15	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	120	THR	CB-CA-C	-7.97	90.08	111.60
1	C	117	ALA	CB-CA-C	7.06	120.69	110.10
1	C	115	PRO	CB-CA-C	-7.03	94.43	112.00
2	B	120	THR	N-CA-C	6.91	129.66	111.00
2	B	85	TRP	N-CA-C	-5.80	95.33	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	2829	0	2794	67	0
1	C	2859	0	2820	87	0
2	B	1045	0	1043	56	0
2	D	999	0	1000	35	0
3	E	34	0	30	1	0
3	F	34	0	30	1	0
4	A	4	0	6	4	0
4	C	8	0	12	8	0
5	C	10	0	4	0	0
6	A	130	0	0	5	0
6	B	30	0	0	3	0
6	C	134	0	0	3	0
6	D	11	0	0	1	0
All	All	8127	0	7739	240	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 15.

The worst 5 of 240 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)
2:B:84:ARG:O	2:B:85:TRP:HD1	1.12	1.23
1:A:80:GLN:HB3	1:A:107:TYR:OH	1.36	1.20
2:B:84:ARG:O	2:B:85:TRP:CD1	1.97	1.18
2:D:114:VAL:HB	2:D:115:PRO:HD2	1.26	1.11
1:A:179:TYR:OH	1:A:182:GLY:HA2	1.56	1.05

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	363/387 (94%)	355 (98%)	8 (2%)	0	100	100
1	C	367/387 (95%)	354 (96%)	13 (4%)	0	100	100
2	B	137/141 (97%)	132 (96%)	4 (3%)	1 (1%)	22	21
2	D	129/141 (92%)	124 (96%)	4 (3%)	1 (1%)	19	17
All	All	996/1056 (94%)	965 (97%)	29 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	THR
2	D	117	ALA

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	293/312 (94%)	286 (98%)	7 (2%)	49	58
1	C	296/312 (95%)	287 (97%)	9 (3%)	41	50
2	B	103/104 (99%)	91 (88%)	12 (12%)	5	3
2	D	100/104 (96%)	90 (90%)	10 (10%)	7	5
All	All	792/832 (95%)	754 (95%)	38 (5%)	25	28

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	35	GLU
2	D	92	LEU
2	D	42	ARG
2	D	86	LYS
2	D	130	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	261	GLN
1	C	375	ASN
2	D	98	GLN
2	D	45	ASN
1	C	302	ASN

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)

6 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	GLC	E	1	3	12,12,12	0.74	0	17,17,17	1.58	4 (23%)
3	GLC	E	2	3	11,11,12	0.75	0	15,15,17	2.39	5 (33%)
3	GLC	E	3	3	11,11,12	1.45	3 (27%)	15,15,17	1.54	2 (13%)
3	GLC	F	1	3	12,12,12	0.75	0	17,17,17	1.17	2 (11%)
3	GLC	F	2	3	11,11,12	0.79	0	15,15,17	0.98	0
3	GLC	F	3	3	11,11,12	1.21	2 (18%)	15,15,17	2.18	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	E	1	3	-	2/2/22/22	0/1/1/1
3	GLC	E	2	3	-	2/2/19/22	0/1/1/1
3	GLC	E	3	3	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1
3	GLC	F	3	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	GLC	C1-C2	2.43	1.57	1.52
3	E	3	GLC	O5-C1	2.43	1.47	1.43
3	E	3	GLC	O5-C5	2.35	1.48	1.43
3	E	3	GLC	C2-C3	2.30	1.55	1.52
3	F	3	GLC	C2-C3	2.06	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	GLC	C1-O5-C5	6.50	120.99	112.19
3	E	2	GLC	C1-O5-C5	5.47	119.60	112.19
3	E	2	GLC	O5-C5-C6	-4.83	99.63	107.20
3	E	3	GLC	C1-O5-C5	3.80	117.34	112.19
3	E	1	GLC	C1-O5-C5	3.72	120.68	113.66

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	GLC	C4-C5-C6-O6
3	E	1	GLC	C4-C5-C6-O6
3	E	2	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6

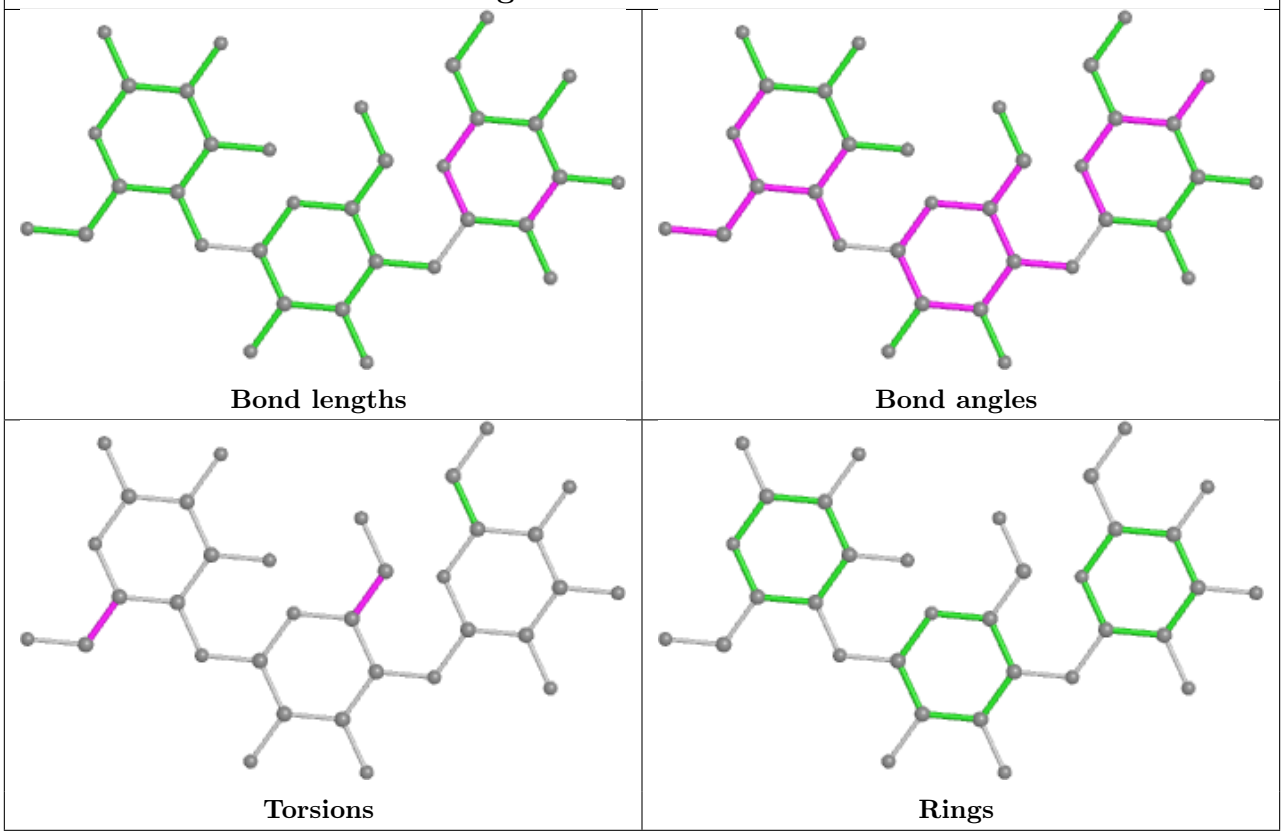
There are no ring outliers.

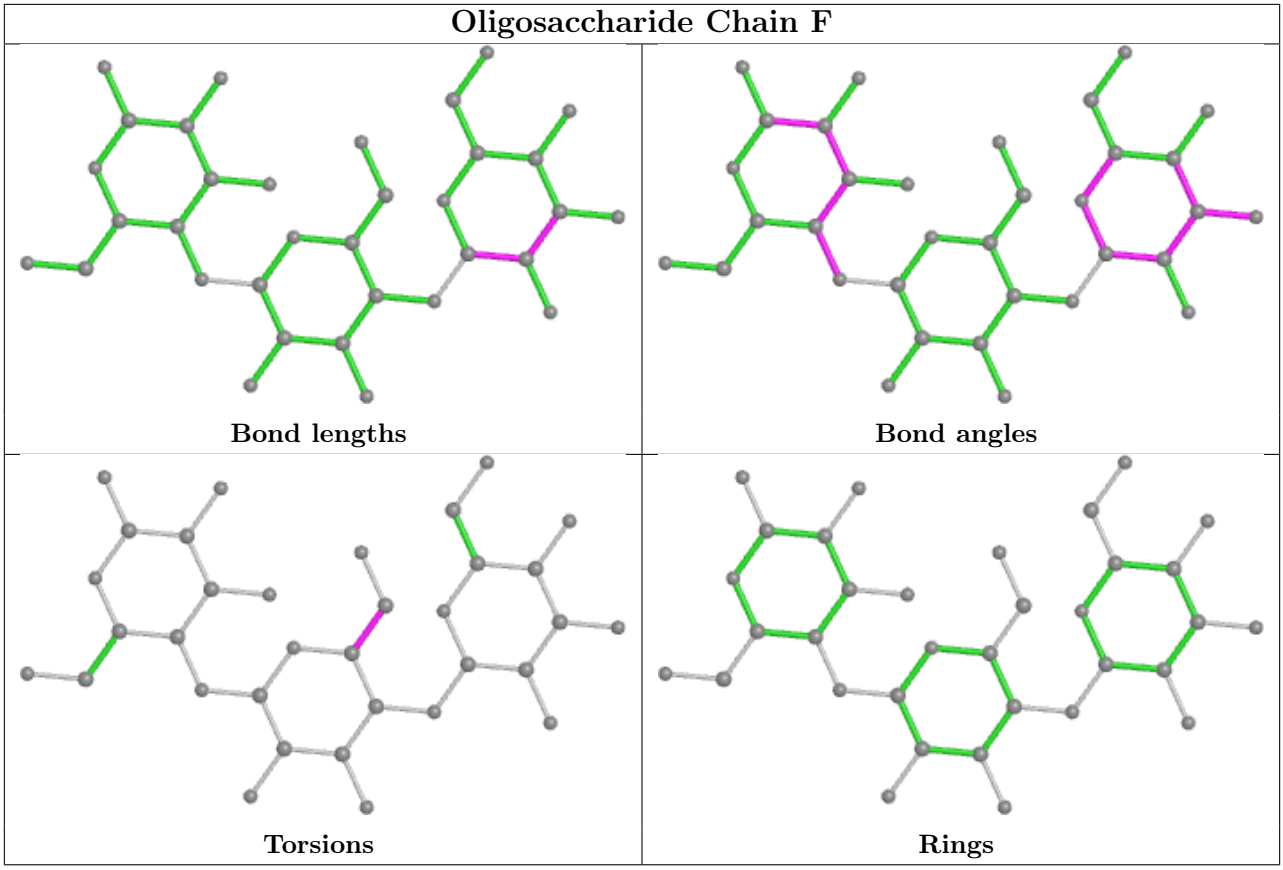
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	GLC	1	0
3	E	3	GLC	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.

Oligosaccharide Chain E





5.6 Ligand geometry (i)

4 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	EDO	C	396	-	3,3,3	0.47	0	2,2,2	0.18	0
5	TAR	C	395	-	9,9,9	1.35	1 (11%)	12,12,12	1.87	3 (25%)
4	EDO	A	2	-	3,3,3	0.30	0	2,2,2	0.93	0
4	EDO	C	3	-	3,3,3	0.33	0	2,2,2	0.27	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	EDO	C	396	-	-	0/1/1/1	-
5	TAR	C	395	-	1/1/4/4	10/12/12/12	-
4	EDO	A	2	-	-	1/1/1/1	-
4	EDO	C	3	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	395	TAR	O3-C3	2.18	1.46	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	395	TAR	O41-C4-C3	3.27	122.11	113.27
5	C	395	TAR	O4-C4-C3	-2.90	114.02	121.63
5	C	395	TAR	O2-C2-C1	-2.67	105.07	110.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	395	TAR	C2

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	395	TAR	O2-C2-C3-O3
5	C	395	TAR	O2-C2-C3-C4
5	C	395	TAR	O3-C3-C4-O4
5	C	395	TAR	O3-C3-C4-O41
5	C	395	TAR	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	EDO	4	0
4	C	3	EDO	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	365/387 (94%)	-0.19	9 (2%)	57	60	6, 15, 25, 34	0
1	C	369/387 (95%)	-0.23	7 (1%)	66	69	8, 14, 25, 37	0
2	B	139/141 (98%)	-0.01	5 (3%)	42	44	14, 20, 30, 38	0
2	D	131/141 (92%)	0.19	9 (6%)	16	18	15, 21, 30, 32	0
All	All	1004/1056 (95%)	-0.13	30 (2%)	50	53	6, 17, 28, 38	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	SER	6.4
1	C	91	LYS	6.1
2	B	121	TYR	5.9
1	C	378	SER	4.8
1	C	92	ALA	3.8

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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
3	GLC	F	3	11/12	0.89	0.15	26,29,32,32	0
3	GLC	E	3	11/12	0.93	0.15	22,26,31,31	0

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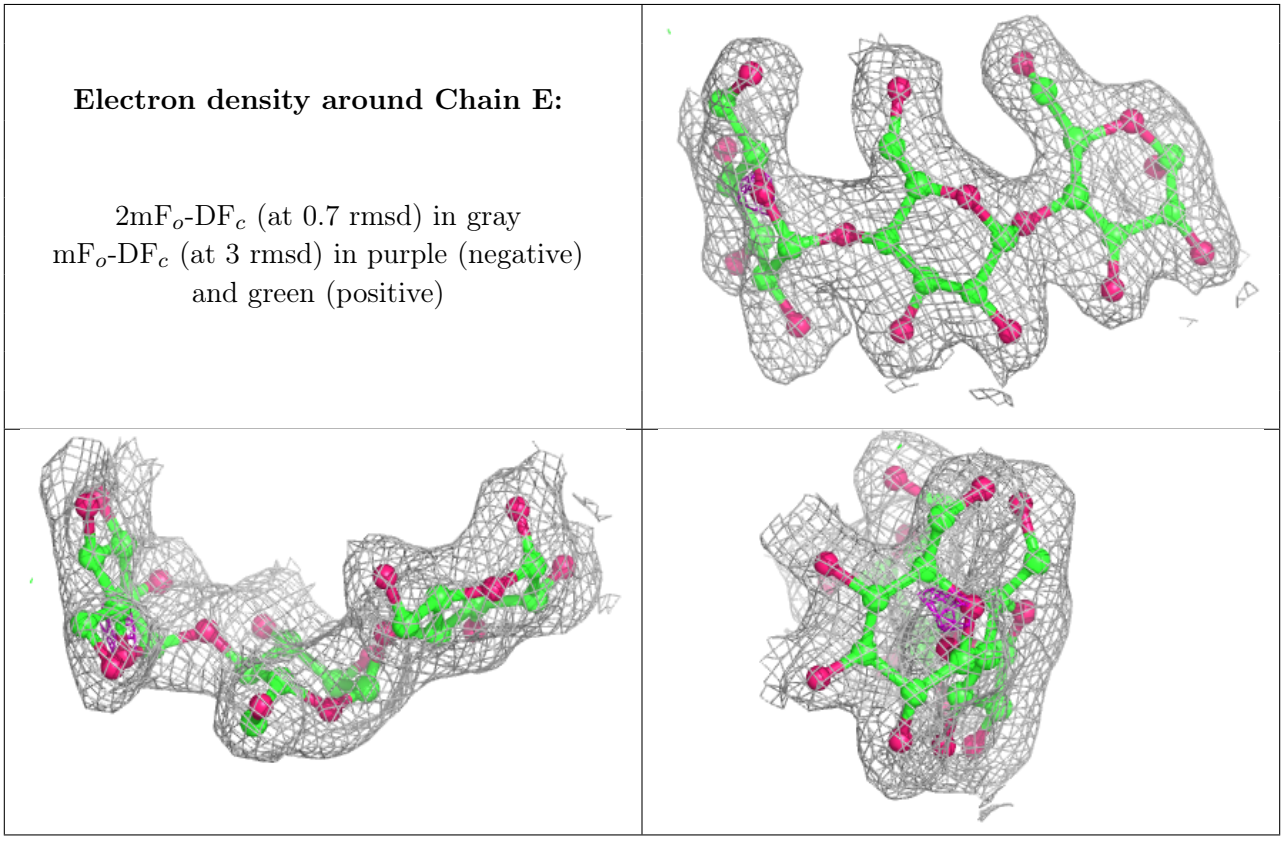
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	F	1	12/12	0.96	0.10	10,16,20,21	0
3	GLC	F	2	11/12	0.97	0.09	15,17,22,23	0
3	GLC	E	1	12/12	0.97	0.12	18,23,27,29	0
3	GLC	E	2	11/12	0.98	0.09	14,19,21,23	0

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.

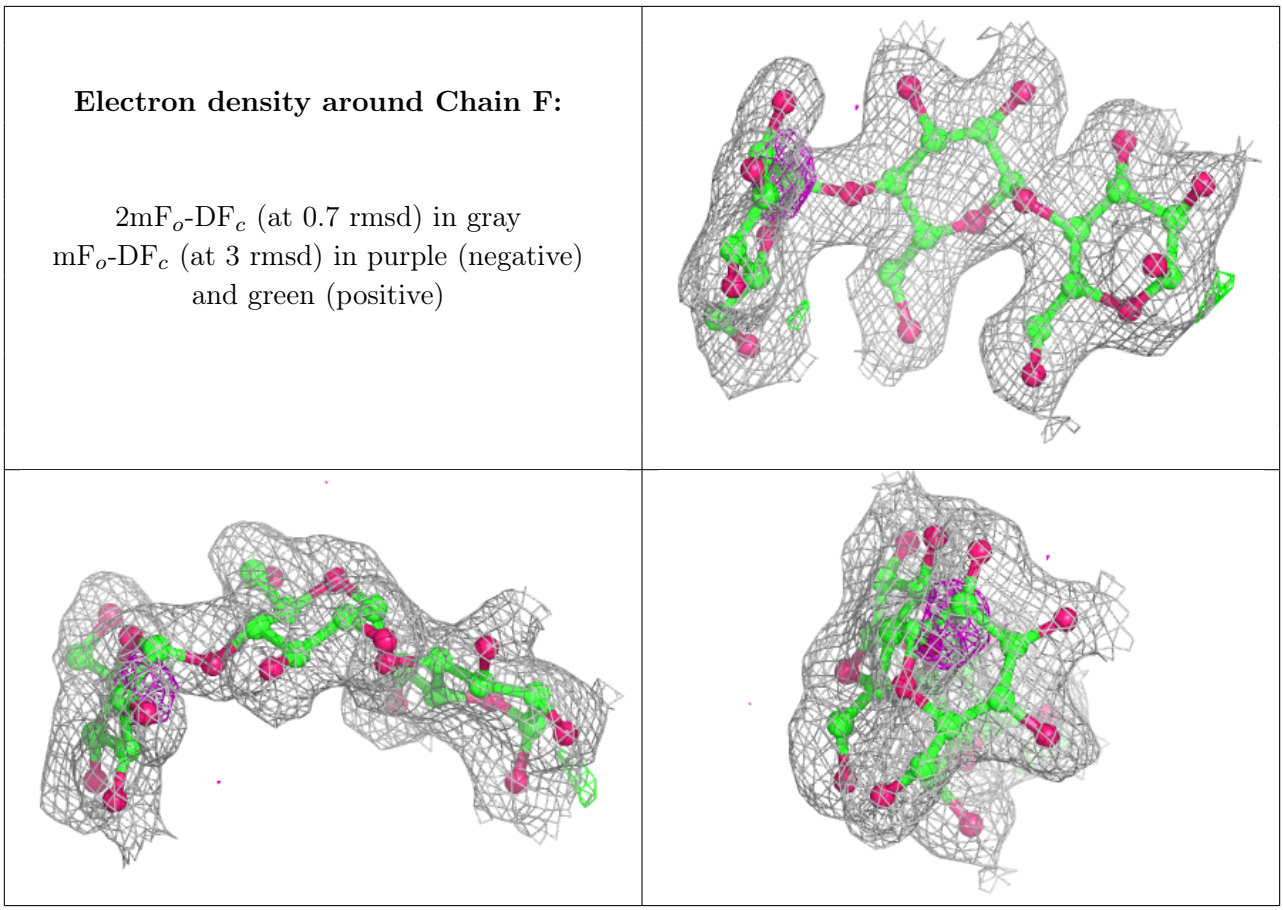
Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
5	TAR	C	395	10/10	0.84	0.20	39,45,47,49	0
4	EDO	C	396	4/4	0.87	0.18	40,44,45,48	0
4	EDO	C	3	4/4	0.92	0.38	29,29,32,33	0
4	EDO	A	2	4/4	0.96	0.11	21,21,25,26	0

6.5 Other polymers

There are no such residues in this entry.