



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2020 – 10:46 AM EST

PDB ID : 6VCA
Title : TB38 complex
Authors : Zhou, Y.F.; Lord, D.M.
Deposited on : 2019-12-20
Resolution : 3.73 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.6
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) : 2.14.6

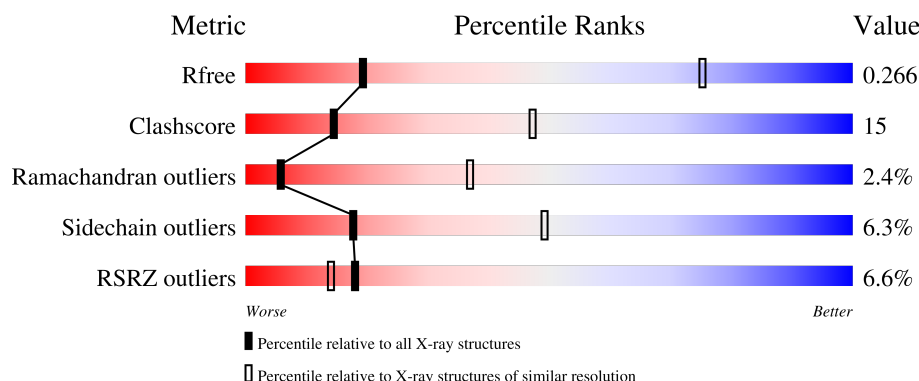
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.73 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	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)

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 ≥ 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	529	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	B	529	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	C	529	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>..</div> </div> </div>
1	D	529	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
2	E	233	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>.. 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	233	
2	K	233	
2	P	233	
3	F	216	
3	J	216	
3	L	216	
3	O	216	
4	G	2	
5	I	3	

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
5	BMA	I	3	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27834 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 5'-nucleotidase, ecto (CD73), isoform CRA_a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	1	0
			4087	2600	700	768	19			
1	B	523	Total	C	N	O	S	0	0	0
			4081	2595	699	768	19			
1	C	523	Total	C	N	O	S	0	0	0
			4071	2589	695	768	19			
1	D	523	Total	C	N	O	S	0	3	0
			4095	2605	701	770	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	HIS	-	expression tag	UNP Q53Z63
A	551	HIS	-	expression tag	UNP Q53Z63
A	552	HIS	-	expression tag	UNP Q53Z63
A	553	HIS	-	expression tag	UNP Q53Z63
A	554	HIS	-	expression tag	UNP Q53Z63
A	555	HIS	-	expression tag	UNP Q53Z63
B	550	HIS	-	expression tag	UNP Q53Z63
B	551	HIS	-	expression tag	UNP Q53Z63
B	552	HIS	-	expression tag	UNP Q53Z63
B	553	HIS	-	expression tag	UNP Q53Z63
B	554	HIS	-	expression tag	UNP Q53Z63
B	555	HIS	-	expression tag	UNP Q53Z63
C	550	HIS	-	expression tag	UNP Q53Z63
C	551	HIS	-	expression tag	UNP Q53Z63
C	552	HIS	-	expression tag	UNP Q53Z63
C	553	HIS	-	expression tag	UNP Q53Z63
C	554	HIS	-	expression tag	UNP Q53Z63
C	555	HIS	-	expression tag	UNP Q53Z63
D	550	HIS	-	expression tag	UNP Q53Z63
D	551	HIS	-	expression tag	UNP Q53Z63
D	552	HIS	-	expression tag	UNP Q53Z63

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Chain	Residue	Modelled	Actual	Comment	Reference
D	553	HIS	-	expression tag	UNP Q53Z63
D	554	HIS	-	expression tag	UNP Q53Z63
D	555	HIS	-	expression tag	UNP Q53Z63

- Molecule 2 is a protein called TB38 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1654	1047	278	322	7			
2	E	219	Total	C	N	O	S	0	1	0
			1649	1043	277	322	7			
2	P	119	Total	C	N	O	S	0	0	0
			928	587	159	177	5			
2	K	220	Total	C	N	O	S	0	0	0
			1654	1047	278	322	7			

- Molecule 3 is a protein called TB38 light chain.

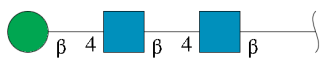
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1573	990	257	321	5			
3	F	212	Total	C	N	O	S	0	1	0
			1575	991	257	322	5			
3	O	110	Total	C	N	O	S	0	0	0
			813	512	132	166	3			
3	J	212	Total	C	N	O	S	0	0	0
			1573	990	257	321	5			

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



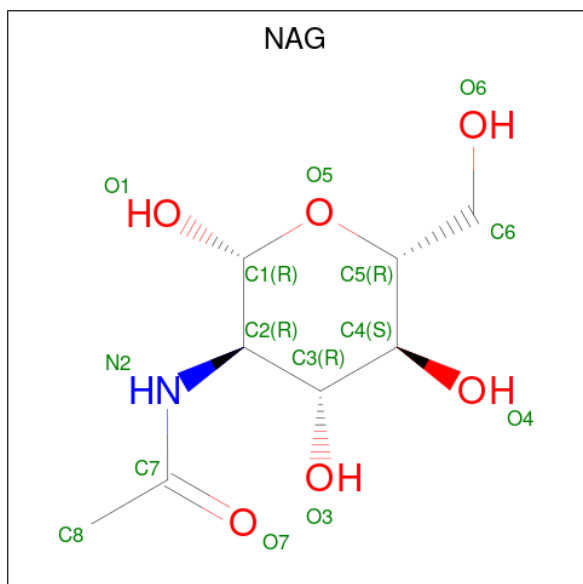
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(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
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

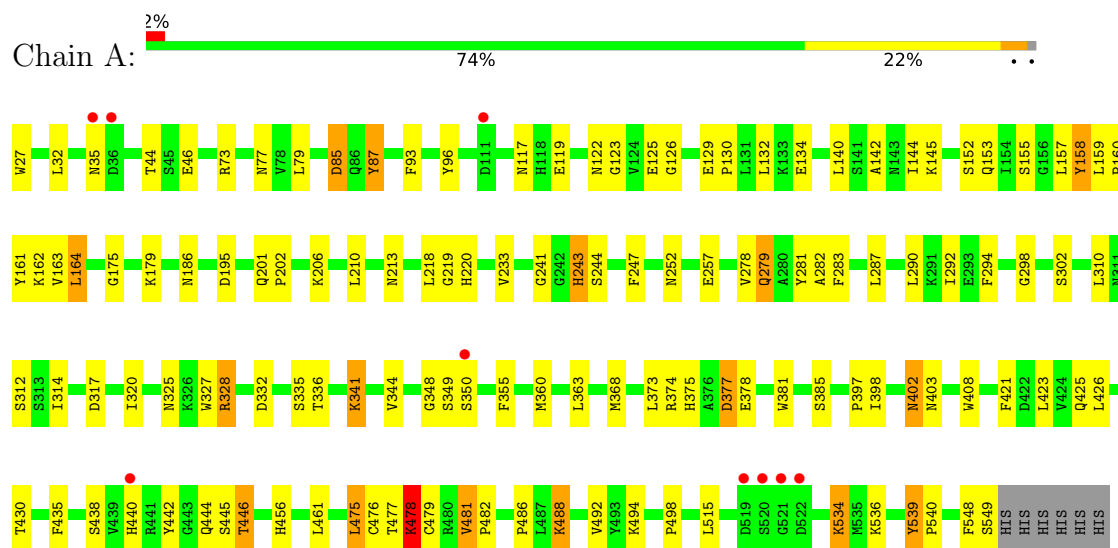


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

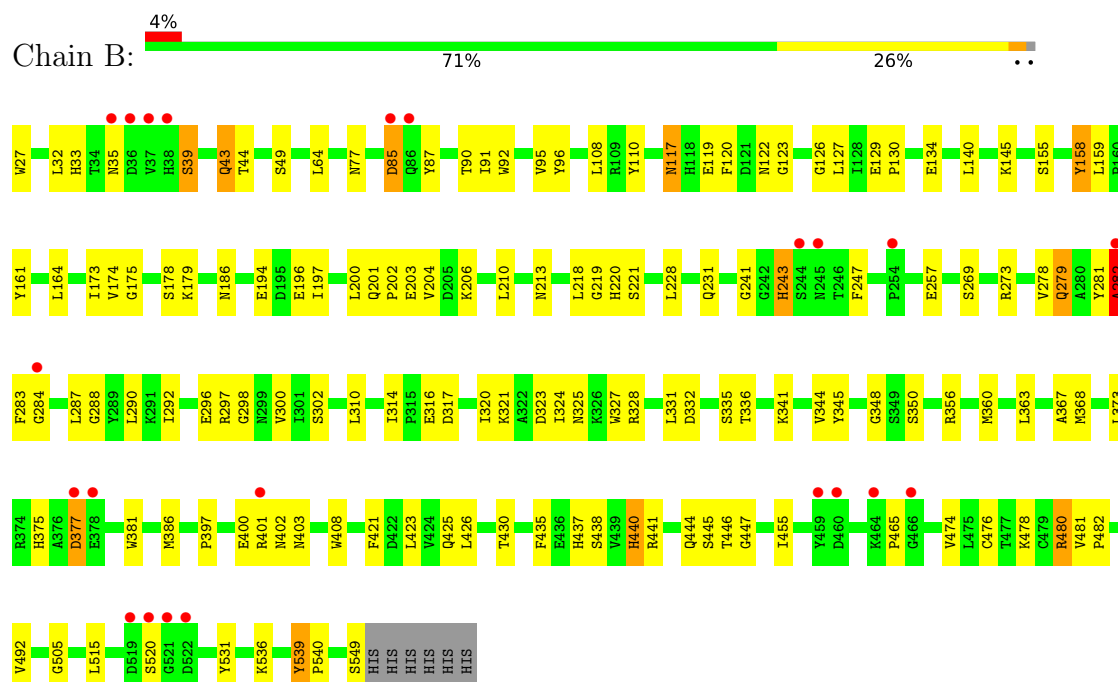
3 Residue-property plots [i](#)

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: 5'-nucleotidase, ecto (CD73), isoform CRA_a



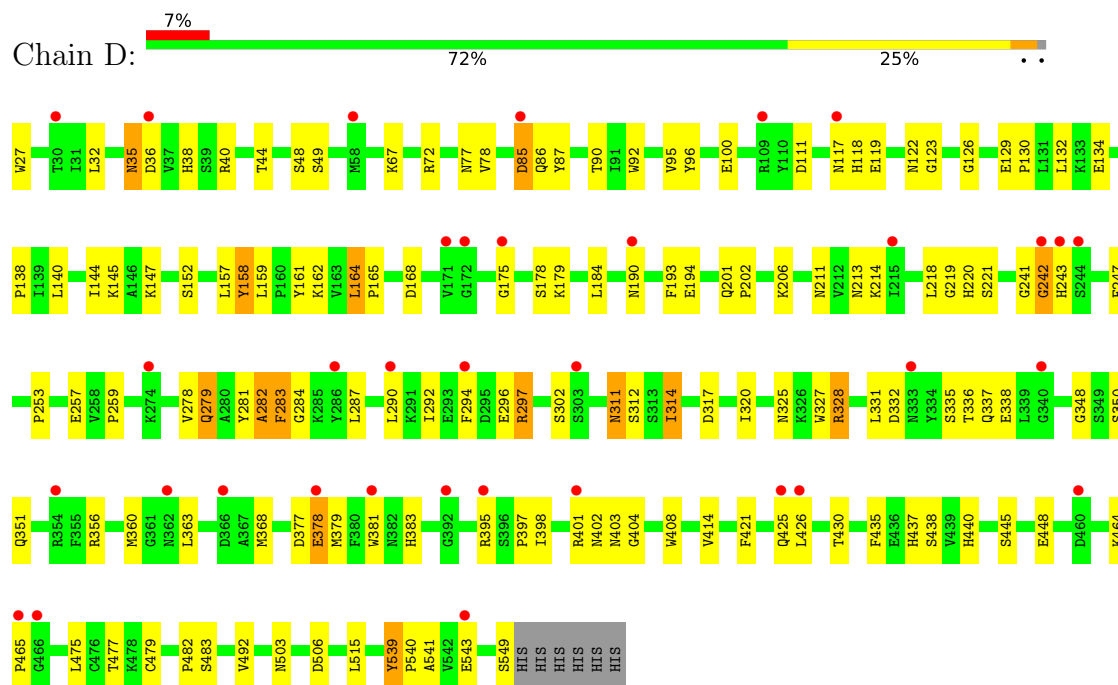
- Molecule 1: 5'-nucleotidase, ecto (CD73), isoform CRA_a



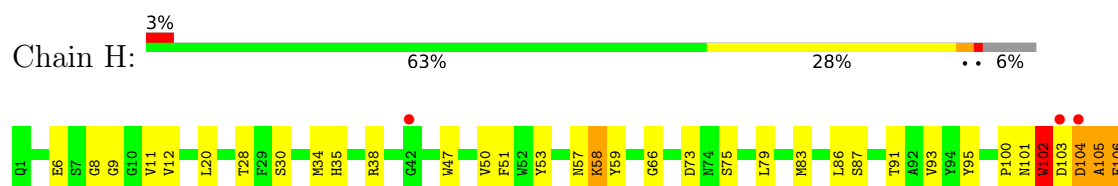
• Molecule 1: 5'-nucleotidase, ecto (CD73), isoform CRA_a



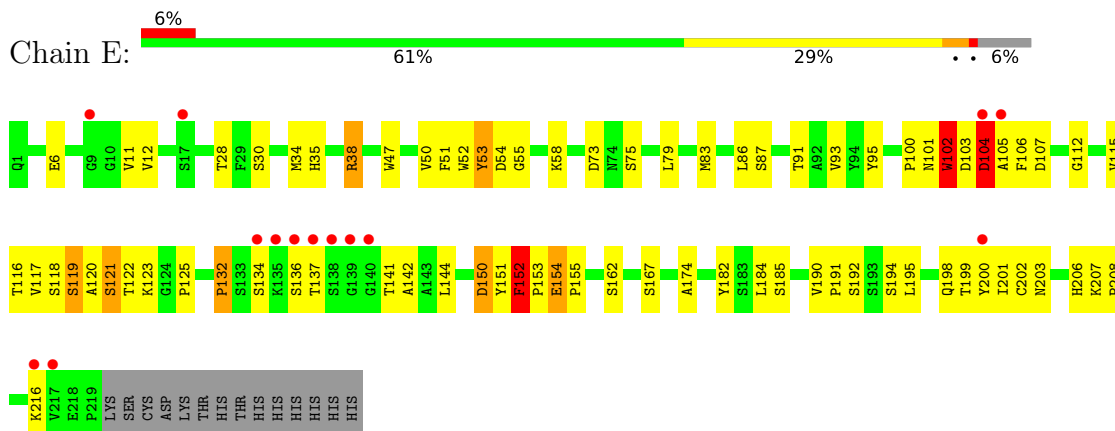
• Molecule 1: 5'-nucleotidase, ecto (CD73), isoform CRA_a



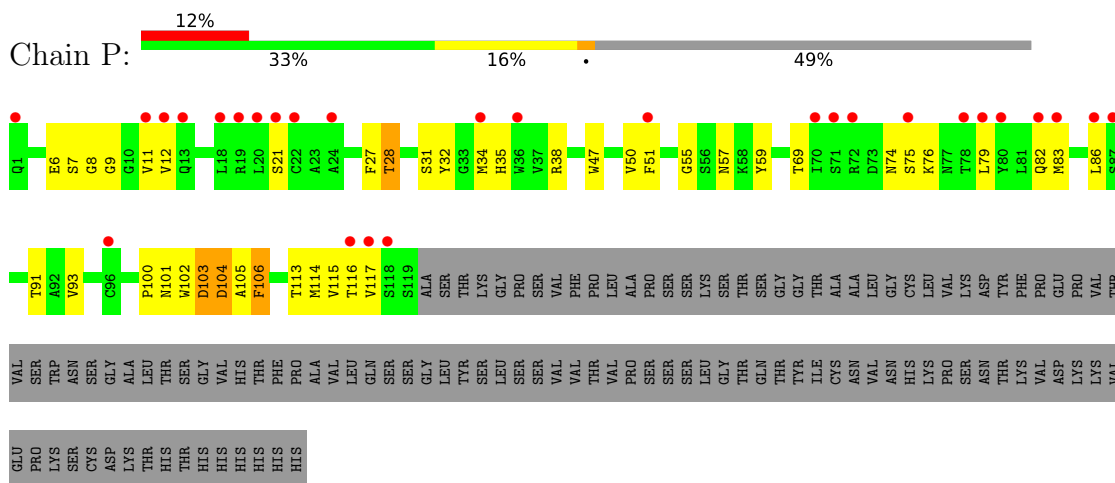
• Molecule 2: TB38 heavy chain



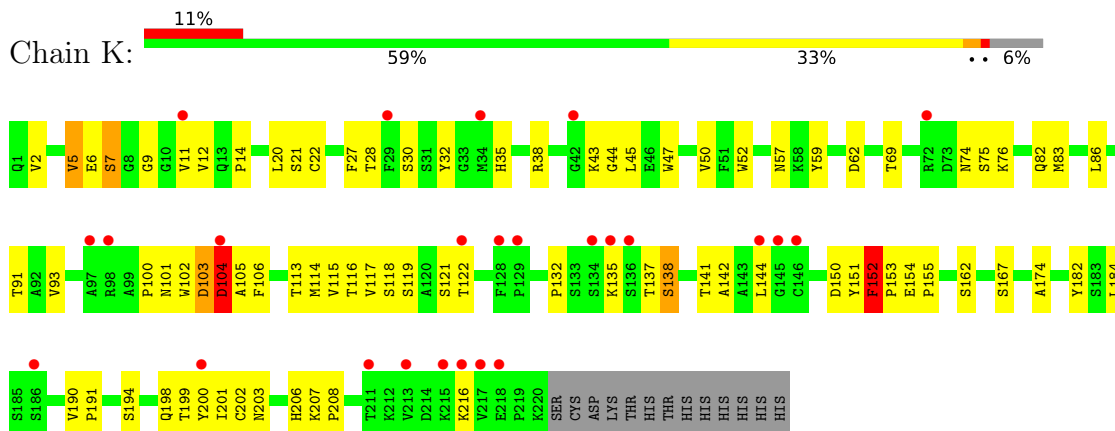
- Molecule 2: TB38 heavy chain



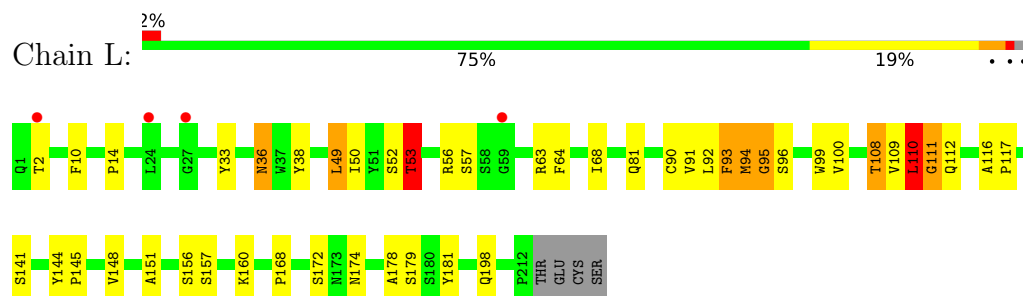
- Molecule 2: TB38 heavy chain



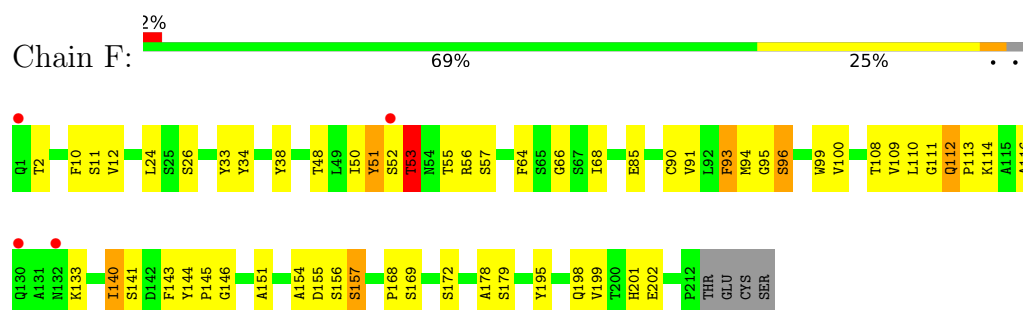
- Molecule 2: TB38 heavy chain



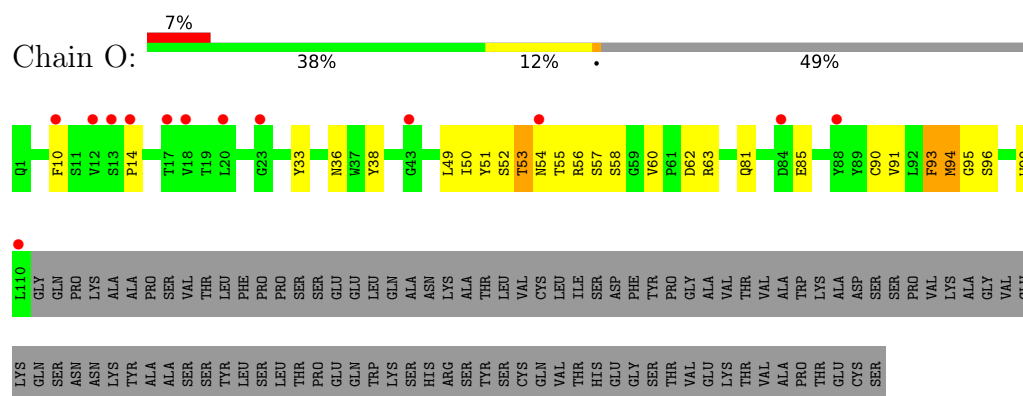
- Molecule 3: TB38 light chain



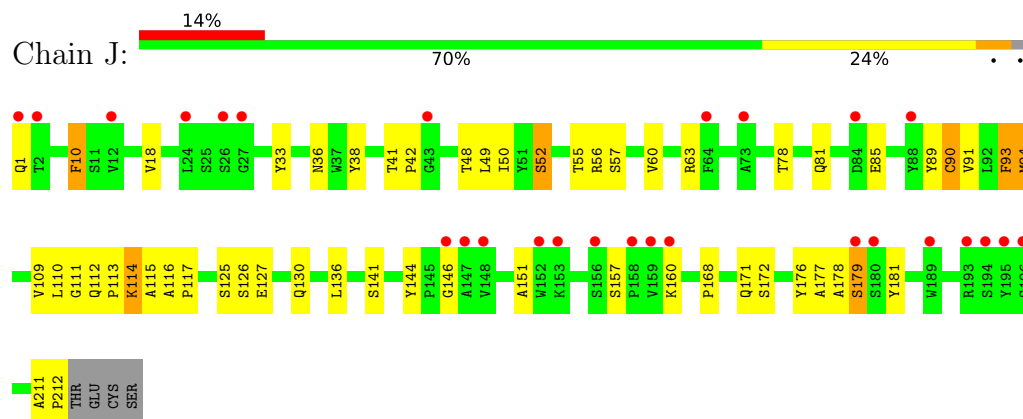
- Molecule 3: TB38 light chain



- Molecule 3: TB38 light chain



- Molecule 3: TB38 light chain



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

Chain G:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2
B1A3

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	236.91Å 336.20Å 222.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.73 39.72 – 3.73	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-3.73) 99.8 (39.72-3.73)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.224 , 0.264 0.229 , 0.266	Depositor DCC
R_{free} test set	4586 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	163.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 168.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27834	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BMA, 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	0.73	1/4176 (0.0%)	0.94	1/5654 (0.0%)
1	B	0.73	0/4167	0.93	1/5643 (0.0%)
1	C	0.72	0/4157	0.89	0/5632
1	D	0.72	0/4190	0.92	1/5674 (0.0%)
2	E	0.79	2/1697 (0.1%)	0.99	4/2314 (0.2%)
2	H	0.80	0/1698	0.99	3/2315 (0.1%)
2	K	0.73	0/1698	0.92	1/2315 (0.0%)
2	P	0.75	0/953	0.93	2/1294 (0.2%)
3	F	0.78	0/1619	0.98	0/2217
3	J	0.73	0/1613	0.90	0/2209
3	L	0.76	0/1613	0.98	0/2209
3	O	0.77	0/832	0.92	0/1137
All	All	0.74	3/28413 (0.0%)	0.94	13/38613 (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
1	B	0	1
1	C	0	1
2	E	0	1
2	H	0	2
2	K	0	1
3	F	0	1
3	L	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	104	ASP	CG-OD2	5.51	1.38	1.25
1	A	378	GLU	CD-OE2	5.17	1.31	1.25
2	E	104	ASP	CB-CG	5.02	1.62	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	104	ASP	CB-CA-C	9.83	130.06	110.40
2	E	104	ASP	CB-CG-OD2	8.91	126.32	118.30
2	H	104	ASP	CB-CA-C	7.64	125.68	110.40
2	P	104	ASP	CB-CA-C	6.22	122.85	110.40
1	D	403	ASN	CB-CA-C	5.92	122.25	110.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	282	ALA	Peptide
1	C	75	GLU	Peptide
2	H	152	PHE	Peptide
2	H	8	GLY	Peptide
3	L	110	LEU	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	4087	0	4079	107	0
1	B	4081	0	4064	129	0
1	C	4071	0	4045	127	0
1	D	4095	0	4088	122	0
2	E	1649	0	1590	81	0
2	H	1654	0	1595	66	0
2	K	1654	0	1595	87	2
2	P	928	0	873	59	0
3	F	1575	0	1516	58	0
3	J	1573	0	1515	49	0
3	L	1573	0	1515	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	813	0	783	31	2
4	G	28	0	25	0	0
5	I	39	0	34	0	0
6	D	14	0	13	2	0
All	All	27834	0	27330	846	2

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 846 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:K:105:ALA:HB1	3:J:36:ASN:ND2	1.28	1.42
2:K:105:ALA:CB	3:J:36:ASN:HD22	1.54	1.20
2:P:105:ALA:HB1	3:O:36:ASN:HD22	0.99	1.16
1:B:145:LYS:NZ	2:H:53:TYR:OH	1.87	1.07
2:H:153:PRO:HG3	2:H:206:HIS:CD2	1.93	1.04

All (2) 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)
3:O:58:SER:O	2:K:138:SER:N[8_455]	1.95	0.25
3:O:58:SER:O	2:K:138:SER:CA[8_455]	1.98	0.22

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	522/529 (99%)	451 (86%)	60 (12%)	11 (2%)	7	40
1	B	521/529 (98%)	454 (87%)	58 (11%)	9 (2%)	9	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	521/529 (98%)	444 (85%)	64 (12%)	13 (2%)	5	36
1	D	524/529 (99%)	456 (87%)	57 (11%)	11 (2%)	7	40
2	E	218/233 (94%)	185 (85%)	27 (12%)	6 (3%)	5	35
2	H	218/233 (94%)	186 (85%)	25 (12%)	7 (3%)	4	32
2	K	218/233 (94%)	187 (86%)	23 (11%)	8 (4%)	3	29
2	P	117/233 (50%)	104 (89%)	10 (8%)	3 (3%)	5	36
3	F	211/216 (98%)	185 (88%)	22 (10%)	4 (2%)	8	42
3	J	210/216 (97%)	184 (88%)	21 (10%)	5 (2%)	6	37
3	L	210/216 (97%)	183 (87%)	23 (11%)	4 (2%)	8	42
3	O	108/216 (50%)	89 (82%)	15 (14%)	4 (4%)	3	29
All	All	3598/3912 (92%)	3108 (86%)	405 (11%)	85 (2%)	6	37

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ASP
1	A	282	ALA
1	A	442	TYR
1	B	85	ASP
1	B	282	ALA

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	451/456 (99%)	425 (94%)	26 (6%)	20	52
1	B	450/456 (99%)	430 (96%)	20 (4%)	28	57
1	C	448/456 (98%)	421 (94%)	27 (6%)	19	51
1	D	453/456 (99%)	429 (95%)	24 (5%)	22	54
2	E	183/197 (93%)	166 (91%)	17 (9%)	9	36
2	H	182/197 (92%)	169 (93%)	13 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	182/197 (92%)	170 (93%)	12 (7%)	16	48
2	P	97/197 (49%)	97 (100%)	0	100	100
3	F	177/182 (97%)	159 (90%)	18 (10%)	7	32
3	J	176/182 (97%)	162 (92%)	14 (8%)	12	42
3	L	176/182 (97%)	158 (90%)	18 (10%)	7	32
3	O	91/182 (50%)	87 (96%)	4 (4%)	28	57
All	All	3066/3340 (92%)	2873 (94%)	193 (6%)	18	49

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	328	ARG
2	H	202	CYS
2	K	203	ASN
1	D	350	SER
2	H	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	456	HIS
1	D	86	GLN
2	K	111	GLN
1	D	35	ASN
1	D	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

5 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	$\# Z > 2$
4	NAG	G	1	1,4	14,14,15	0.27	0	17,19,21	0.80	0
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	0.68	0
5	NAG	I	1	1,5	14,14,15	0.29	0	17,19,21	0.92	0
5	NAG	I	2	5	14,14,15	0.28	0	17,19,21	0.61	0
5	BMA	I	3	5	11,11,12	0.26	0	15,15,17	0.83	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	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	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
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
6	NAG	D	601	1	14,14,15	0.82	1 (7%)	17,19,21	2.32	5 (29%)

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
6	NAG	D	601	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	601	NAG	C1-C2	2.29	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601	NAG	C1-O5-C5	5.33	119.42	112.19
6	D	601	NAG	O5-C5-C6	4.72	114.61	107.20
6	D	601	NAG	C4-C3-C2	-3.35	106.11	111.02
6	D	601	NAG	C2-N2-C7	2.80	126.88	122.90
6	D	601	NAG	O7-C7-N2	2.16	125.93	121.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	601	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	601	NAG	2	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, 95th 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	523/529 (98%)	0.03	9 (1%) 70 64	107, 158, 211, 284	0
1	B	523/529 (98%)	0.25	22 (4%) 36 31	91, 159, 213, 273	0
1	C	523/529 (98%)	0.44	44 (8%) 11 10	150, 218, 269, 445	0
1	D	523/529 (98%)	0.38	35 (6%) 17 14	154, 213, 265, 425	0
2	E	219/233 (93%)	0.45	14 (6%) 19 15	108, 191, 263, 362	0
2	H	220/233 (94%)	0.20	8 (3%) 42 36	102, 160, 233, 333	0
2	K	220/233 (94%)	0.66	25 (11%) 5 5	181, 241, 311, 489	0
2	P	119/233 (51%)	1.09	28 (23%) 0 0	224, 270, 327, 353	0
3	F	212/216 (98%)	0.01	4 (1%) 66 61	114, 171, 233, 265	0
3	J	212/216 (98%)	0.71	30 (14%) 2 3	174, 238, 296, 321	0
3	L	212/216 (98%)	0.18	4 (1%) 66 61	96, 160, 212, 251	0
3	O	110/216 (50%)	0.74	15 (13%) 3 3	192, 243, 293, 343	0
All	All	3616/3912 (92%)	0.35	238 (6%) 18 14	91, 194, 275, 489	0

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	136	SER	9.9
2	K	217	VAL	9.9
2	H	136	SER	9.4
2	E	139	GLY	9.0
2	E	138	SER	7.2

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, 95th 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	BMA	I	3	11/12	0.74	0.54	202,268,299,306	0
4	NAG	G	2	14/15	0.83	0.27	209,248,270,287	0
5	NAG	I	2	14/15	0.83	0.48	198,224,271,328	0
5	NAG	I	1	14/15	0.85	0.47	172,206,232,244	0
4	NAG	G	1	14/15	0.95	0.22	157,195,224,241	0

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, 95th 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
6	NAG	D	601	14/15	0.81	0.21	155,229,256,274	0

6.5 Other polymers [i](#)

There are no such residues in this entry.