



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:58 PM UTC

PDB ID : 2NY3 / pdb_00002ny3
Title : HIV-1 gp120 Envelope Glycoprotein (K231C, T257S, E267C, S334A, S375W)
Complexed with CD4 and Antibody 17b
Authors : Zhou, T.; Xu, L.; Dey, B.; Hessel, A.J.; Van Ryk, D.; Xiang, S.H.; Yang, X.;
Zhang, M.Y.; Zwick, M.B.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Sodroski,
J.; Wyatt, R.; Nabel, G.J.; Kwong, P.D.
Deposited on : 2006-11-20
Resolution : 2.00 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

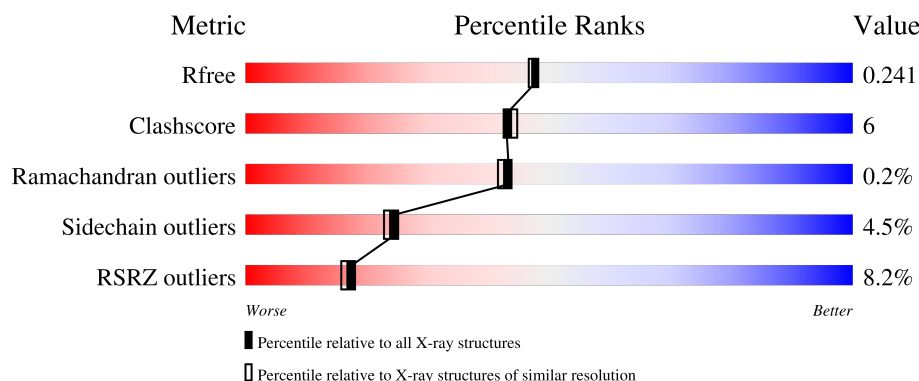
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	317	13% 86% 9% ..
2	B	184	9% 76% 19% ..
3	C	214	2% 88% 12% ..
4	D	229	6% 85% 10% ..

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Mol	Chain	Length	Quality of chain
5	E	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7974 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 ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2357	1480	411	444	22			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1412	885	247	276	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	MET	-	insertion	UNP P01730

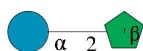
- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	223	Total	C	N	O	S	0	2	0
			1689	1068	285	331	5			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	2	Total	C	O	0	0	0
			23	12	11			

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



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

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

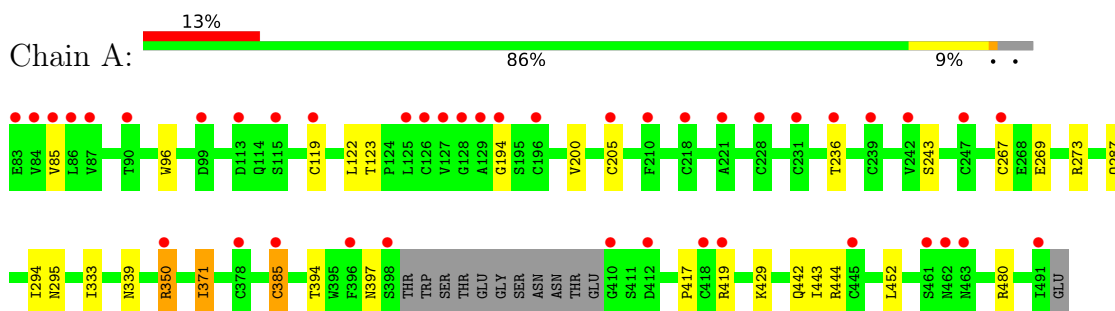
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	215	Total	O	0	0
			215	215		
7	B	99	Total	O	0	0
			99	99		
7	C	162	Total	O	0	0
			162	162		
7	D	189	Total	O	0	0
			189	189		

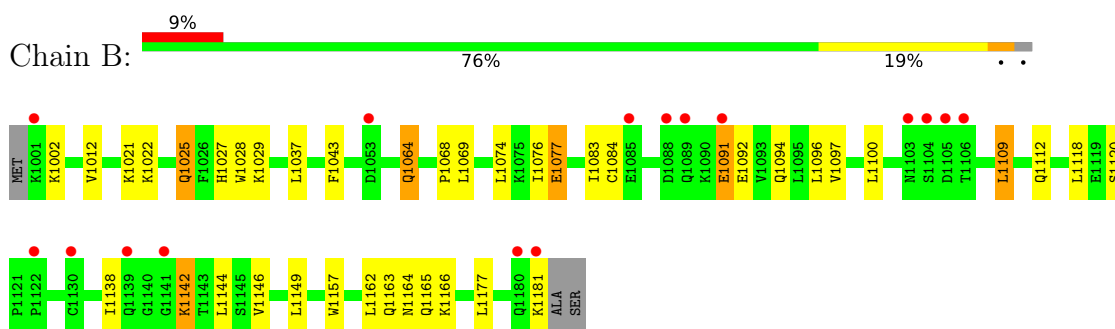
3 Residue-property plots [i](#)

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.

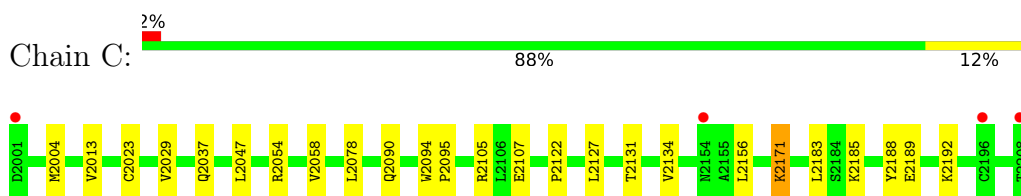
- Molecule 1: ENVELOPE GLYCOPROTEIN GP120



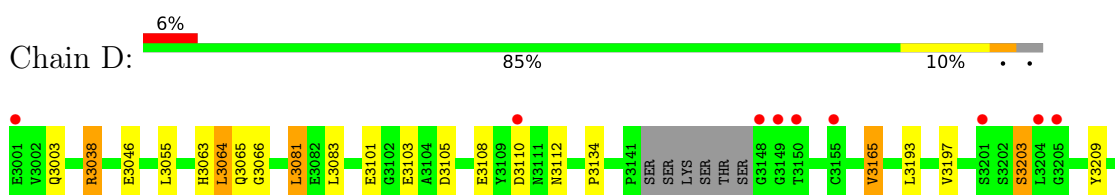
- Molecule 2: T-cell surface glycoprotein CD4



- Molecule 3: ANTIBODY 17B, LIGHT CHAIN



- Molecule 4: ANTIBODY 17B, HEAVY CHAIN





- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.74Å 88.20Å 197.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.11 – 2.00 44.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (44.11-2.00) 91.6 (44.11-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.243 0.202 , 0.241	Depositor DCC
R_{free} test set	3926 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7974	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/2405	0.70	0/3263
2	B	0.35	0/1432	0.65	0/1930
3	C	0.42	1/1683 (0.1%)	0.72	0/2288
4	D	0.40	0/1740	0.69	0/2370
All	All	0.40	1/7260 (0.0%)	0.69	0/9851

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2192	LYS	CE-NZ	5.06	1.64	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2357	0	2296	20	0
2	B	1412	0	1441	33	0
3	C	1646	0	1590	13	0
4	D	1689	0	1650	23	0
5	E	23	0	21	1	0
6	A	182	0	169	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	215	0	0	7	0
7	B	99	0	0	12	0
7	C	162	0	0	1	0
7	D	189	0	0	6	0
All	All	7974	0	7167	89	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 6.

All (89) 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)
4:D:3215:HIS:HB3	4:D:3220:THR:HG22	1.33	1.05
2:B:1068:PRO:HA	7:B:316:HOH:O	1.57	1.04
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.33	0.93
2:B:1025:GLN:HG2	7:B:153:HOH:O	1.69	0.91
1:A:419:ARG:NH2	4:D:3103:GLU:OE2	2.06	0.89
4:D:3003:GLN:OE1	7:D:636:HOH:O	1.94	0.85
4:D:3065:GLN:NE2	7:D:36:HOH:O	2.11	0.84
1:A:350:ARG:HH11	1:A:350:ARG:CG	1.95	0.79
4:D:3046:GLU:OE2	4:D:3063[A]:HIS:NE2	2.15	0.79
2:B:1076:ILE:HD12	7:B:173:HOH:O	1.84	0.76
4:D:3112:ASN:ND2	7:D:506:HOH:O	2.20	0.75
4:D:3215:HIS:HB3	4:D:3220:THR:CG2	2.15	0.75
1:A:480:ARG:NH2	7:A:1093:HOH:O	2.21	0.73
2:B:1097:VAL:O	7:B:173:HOH:O	2.06	0.72
2:B:1027:HIS:CD2	7:B:501:HOH:O	2.41	0.71
4:D:3101:GLU:HA	7:D:506:HOH:O	1.90	0.70
2:B:1028:TRP:HZ2	7:B:316:HOH:O	1.76	0.69
6:A:734:NAG:O7	7:A:1163:HOH:O	2.08	0.69
4:D:3134:PRO:HD2	4:D:3220:THR:HG21	1.76	0.67
1:A:123:THR:HG21	1:A:429:LYS:HE3	1.76	0.67
4:D:3110:ASP:HB2	7:D:506:HOH:O	1.95	0.66
2:B:1029:LYS:HG2	7:B:501:HOH:O	1.95	0.65
1:A:119:CYS:N	1:A:205:CYS:SG	2.70	0.65
2:B:1164:ASN:O	2:B:1166:LYS:HD2	1.99	0.63
2:B:1029:LYS:CG	7:B:501:HOH:O	2.46	0.62
2:B:1120:SER:HA	7:B:173:HOH:O	2.01	0.61
4:D:3063[A]:HIS:CD2	4:D:3064:LEU:HD13	2.37	0.59
4:D:3063[A]:HIS:HD2	4:D:3064:LEU:HD13	1.68	0.59
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2094:TRP:HA	3:C:2095:PRO:C	2.29	0.56
3:C:2188:TYR:CZ	3:C:2213:ARG:HG3	2.40	0.56
4:D:3063[A]:HIS:CE1	5:E:2:FRU:O6	2.58	0.56
2:B:1083:ILE:HG13	2:B:1092:GLU:HG3	1.87	0.56
6:A:762:NAG:O4	7:A:1141:HOH:O	2.07	0.56
2:B:1157:TRP:HB3	7:B:527:HOH:O	2.05	0.56
1:A:295:ASN:HD22	6:A:795:NAG:H83	1.72	0.55
1:A:122:LEU:HD22	1:A:200:VAL:HG22	1.88	0.55
3:C:2171:LYS:HA	3:C:2171:LYS:HE3	1.89	0.54
2:B:1142:LYS:NZ	2:B:1142:LYS:HA	2.24	0.53
3:C:2029:VAL:HG11	3:C:2090:GLN:HG2	1.91	0.52
4:D:3066:GLY:HA3	7:D:254:HOH:O	2.09	0.52
3:C:2185:LYS:HE2	3:C:2189:GLU:OE2	2.10	0.52
4:D:3081:LEU:HD13	4:D:3081:LEU:C	2.35	0.52
2:B:1084:CYS:HB3	2:B:1091:GLU:HG3	1.93	0.51
2:B:1142:LYS:HA	2:B:1142:LYS:HZ2	1.75	0.51
2:B:1120:SER:OG	2:B:1142:LYS:HE2	2.10	0.51
2:B:1138:ILE:HG21	2:B:1146:VAL:HG22	1.93	0.50
3:C:2029:VAL:HG11	3:C:2090:GLN:CG	2.41	0.50
4:D:3038:ARG:HD2	4:D:3046:GLU:OE1	2.12	0.50
3:C:2037:GLN:HB2	3:C:2047:LEU:HD11	1.93	0.49
3:C:2054:ARG:HG2	3:C:2058:VAL:HB	1.94	0.49
3:C:2004:MET:SD	3:C:2090:GLN:HB2	2.53	0.49
1:A:394:THR:HG22	1:A:397:ASN:HB2	1.95	0.48
2:B:1029:LYS:HG3	7:B:501:HOH:O	2.13	0.47
1:A:385:CYS:SG	1:A:417:PRO:O	2.73	0.47
3:C:2122:PRO:HD3	3:C:2134:VAL:HG22	1.98	0.46
3:C:2105:ARG:NH1	7:C:168:HOH:O	2.49	0.45
2:B:1012:VAL:HB	2:B:1074:LEU:HD11	1.97	0.45
2:B:1077:GLU:H	2:B:1077:GLU:CD	2.24	0.45
2:B:1094:GLN:HE21	2:B:1096:LEU:HD21	1.82	0.45
4:D:3193:LEU:C	4:D:3193:LEU:HD12	2.42	0.45
1:A:273:ARG:NH2	1:A:287:GLN:OE1	2.49	0.45
2:B:1021:LYS:HE3	2:B:1064:GLN:OE1	2.17	0.44
1:A:350:ARG:CG	1:A:350:ARG:NH1	2.62	0.44
2:B:1181:LYS:HB3	2:B:1181:LYS:HE3	1.84	0.44
4:D:3038:ARG:HG3	4:D:3046:GLU:HB3	2.00	0.44
4:D:3105:ASP:OD1	4:D:3105:ASP:N	2.51	0.44
1:A:371:ILE:HG12	2:B:1043:PHE:HB3	2.00	0.43
3:C:2004:MET:HE3	3:C:2023:CYS:SG	2.57	0.43
1:A:480:ARG:NE	7:A:1155:HOH:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3203:SER:OG	4:D:3209:TYR:OH	2.34	0.43
4:D:3165:VAL:CG1	4:D:3193:LEU:HD21	2.49	0.42
2:B:1109:LEU:HB2	2:B:1112:GLN:CD	2.45	0.42
2:B:1162:LEU:HD23	2:B:1163:GLN:N	2.34	0.42
4:D:3216:LYS:N	4:D:3217:PRO:CD	2.83	0.42
1:A:269:GLU:HB2	7:A:1161:HOH:O	2.20	0.42
1:A:442:GLN:HG2	1:A:444:ARG:HH12	1.85	0.42
2:B:1027:HIS:HD2	7:B:501:HOH:O	1.93	0.41
2:B:1138:ILE:HD12	2:B:1144:LEU:HB3	2.01	0.41
2:B:1164:ASN:C	2:B:1166:LYS:H	2.28	0.41
1:A:96:TRP:CD1	1:A:236:THR:HG21	2.56	0.41
1:A:444:ARG:HG3	7:A:1074:HOH:O	2.20	0.41
2:B:1118:LEU:O	2:B:1142:LYS:HE3	2.21	0.41
1:A:85:VAL:HA	1:A:243:SER:HB3	2.03	0.41
2:B:1164:ASN:O	2:B:1165:GLN:HB2	2.20	0.40
2:B:1118:LEU:HD23	2:B:1142:LYS:NZ	2.37	0.40
3:C:2013:VAL:CG1	3:C:2078:LEU:HD12	2.51	0.40
7:A:1106:HOH:O	4:D:3108:GLU:HB2	2.21	0.40
2:B:1021:LYS:NZ	2:B:1064:GLN:HG3	2.36	0.40

There are no symmetry-related clashes.

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	301/317 (95%)	283 (94%)	17 (6%)	1 (0%)	36	35
2	B	179/184 (97%)	174 (97%)	5 (3%)	0	100	100
3	C	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
4	D	221/229 (96%)	216 (98%)	4 (2%)	1 (0%)	24	21
All	All	913/944 (97%)	878 (96%)	33 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
4	D	3228	PRO

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	269/280 (96%)	262 (97%)	7 (3%)	40	44
2	B	164/166 (99%)	151 (92%)	13 (8%)	11	8
3	C	184/184 (100%)	178 (97%)	6 (3%)	33	34
4	D	189/193 (98%)	179 (95%)	10 (5%)	20	18
All	All	806/823 (98%)	770 (96%)	36 (4%)	24	23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	CYS
1	A	339	ASN
1	A	350	ARG
1	A	371	ILE
1	A	385	CYS
1	A	443	ILE
1	A	452	LEU
2	B	1002	LYS
2	B	1022	LYS
2	B	1025	GLN
2	B	1037	LEU
2	B	1064	GLN
2	B	1069	LEU
2	B	1077	GLU
2	B	1091	GLU
2	B	1100	LEU
2	B	1109	LEU
2	B	1142	LYS

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Mol	Chain	Res	Type
2	B	1149	LEU
2	B	1177	LEU
3	C	2107	GLU
3	C	2127	LEU
3	C	2131	THR
3	C	2156	LEU
3	C	2171	LYS
3	C	2183	LEU
4	D	3038	ARG
4	D	3055	LEU
4	D	3064	LEU
4	D	3081	LEU
4	D	3083	LEU
4	D	3165	VAL
4	D	3197	VAL
4	D	3203	SER
4	D	3220	THR
4	D	3221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	103	GLN
1	A	332	ASN
1	A	352	GLN
1	A	355	ASN
1	A	377	ASN
2	B	1094	GLN
2	B	1163	GLN
2	B	1164	ASN
3	C	2038	GLN
3	C	2102	GLN
3	C	2191	HIS
4	D	3003	GLN
4	D	3039	GLN

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 ⓘ

2 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	$\# Z > 2$
5	GLC	E	1	5	11,11,12	0.58	0	15,15,17	0.58	0
5	FRU	E	2	5	11,12,12	0.53	0	10,18,18	0.85	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
5	GLC	E	1	5	-	0/2/19/22	0/1/1/1
5	FRU	E	2	5	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

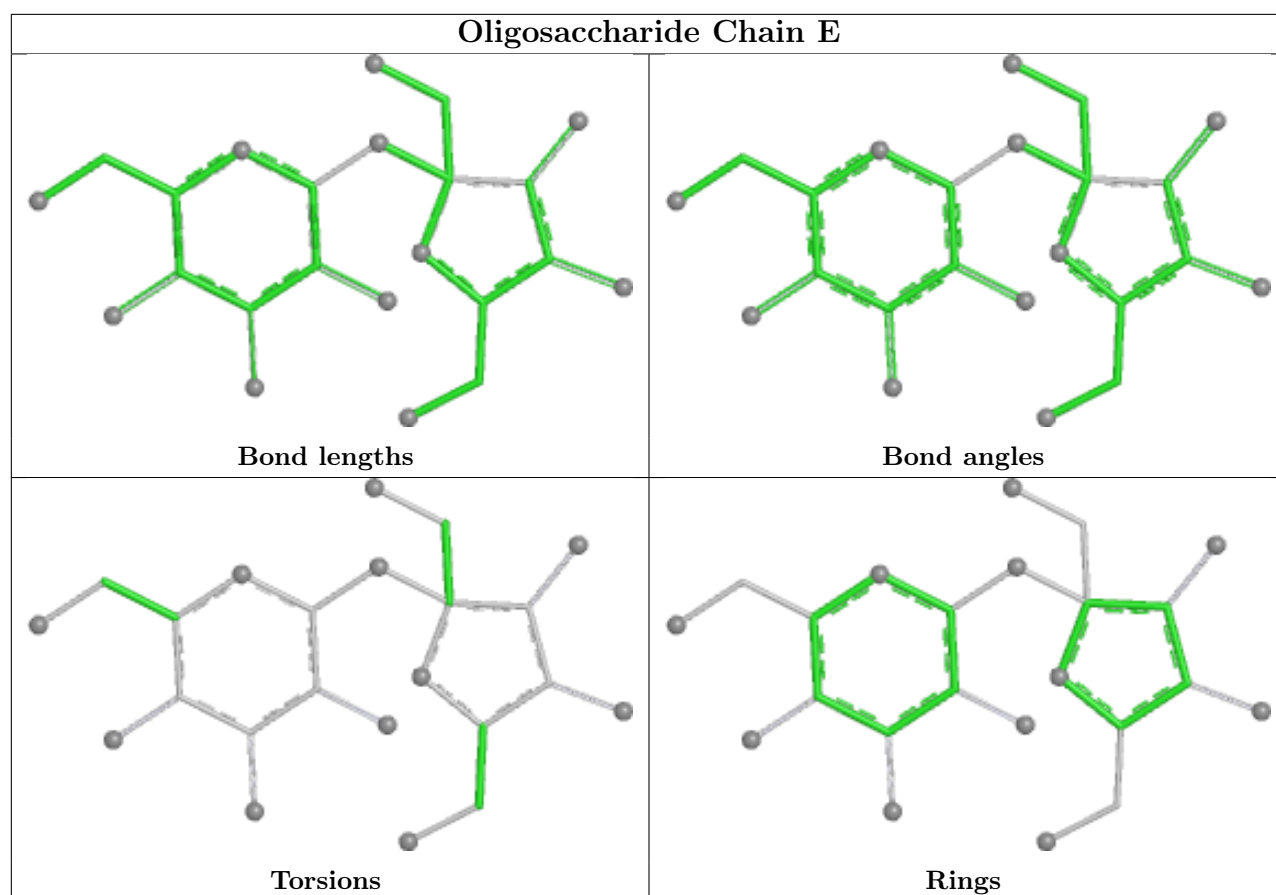
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	FRU	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](#)

13 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	$\# Z > 2$
6	NAG	A	730	1	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
6	NAG	A	892	1	14,14,15	0.57	0	17,19,21	0.81	0
6	NAG	A	734	1	14,14,15	0.53	0	17,19,21	1.99	4 (23%)
6	NAG	A	588	1	14,14,15	0.52	0	17,19,21	0.71	0
6	NAG	A	741	1	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
6	NAG	A	697	1	14,14,15	0.44	0	17,19,21	0.86	0
6	NAG	A	776	1	14,14,15	0.52	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	789	1	14,14,15	0.55	0	17,19,21	0.70	0
6	NAG	A	762	1	14,14,15	0.56	0	17,19,21	0.87	0
6	NAG	A	839	1	14,14,15	0.72	0	17,19,21	1.31	1 (5%)
6	NAG	A	948	1	14,14,15	0.48	0	17,19,21	0.81	0
6	NAG	A	795	1	14,14,15	0.51	0	17,19,21	0.78	0
6	NAG	A	886	1	14,14,15	0.49	0	17,19,21	0.57	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
6	NAG	A	730	1	-	4/6/23/26	0/1/1/1
6	NAG	A	892	1	-	2/6/23/26	0/1/1/1
6	NAG	A	734	1	-	5/6/23/26	0/1/1/1
6	NAG	A	588	1	-	5/6/23/26	0/1/1/1
6	NAG	A	741	1	-	4/6/23/26	0/1/1/1
6	NAG	A	697	1	-	4/6/23/26	0/1/1/1
6	NAG	A	776	1	-	0/6/23/26	0/1/1/1
6	NAG	A	789	1	-	1/6/23/26	0/1/1/1
6	NAG	A	762	1	-	0/6/23/26	0/1/1/1
6	NAG	A	839	1	-	3/6/23/26	0/1/1/1
6	NAG	A	948	1	-	0/6/23/26	0/1/1/1
6	NAG	A	795	1	-	2/6/23/26	0/1/1/1
6	NAG	A	886	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	734	NAG	C1-O5-C5	6.05	120.30	112.19
6	A	839	NAG	C4-C3-C2	4.20	117.18	111.02
6	A	734	NAG	C4-C3-C2	-3.30	106.19	111.02
6	A	734	NAG	O5-C1-C2	3.05	116.01	111.29
6	A	730	NAG	C4-C3-C2	2.62	114.86	111.02
6	A	734	NAG	C3-C4-C5	-2.34	106.00	110.23
6	A	741	NAG	C4-C3-C2	2.27	114.34	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	588	NAG	C1-C2-N2-C7
6	A	697	NAG	C8-C7-N2-C2
6	A	697	NAG	O7-C7-N2-C2
6	A	730	NAG	C8-C7-N2-C2
6	A	730	NAG	O7-C7-N2-C2
6	A	734	NAG	C1-C2-N2-C7
6	A	734	NAG	C8-C7-N2-C2
6	A	734	NAG	O7-C7-N2-C2
6	A	741	NAG	C8-C7-N2-C2
6	A	741	NAG	O7-C7-N2-C2
6	A	839	NAG	C3-C2-N2-C7
6	A	839	NAG	C8-C7-N2-C2
6	A	839	NAG	O7-C7-N2-C2
6	A	697	NAG	O5-C5-C6-O6
6	A	730	NAG	O5-C5-C6-O6
6	A	697	NAG	C4-C5-C6-O6
6	A	734	NAG	O5-C5-C6-O6
6	A	892	NAG	O5-C5-C6-O6
6	A	730	NAG	C4-C5-C6-O6
6	A	741	NAG	O5-C5-C6-O6
6	A	741	NAG	C4-C5-C6-O6
6	A	588	NAG	C8-C7-N2-C2
6	A	795	NAG	C8-C7-N2-C2
6	A	795	NAG	O7-C7-N2-C2
6	A	892	NAG	C4-C5-C6-O6
6	A	588	NAG	C4-C5-C6-O6
6	A	588	NAG	O5-C5-C6-O6
6	A	734	NAG	C4-C5-C6-O6
6	A	588	NAG	O7-C7-N2-C2
6	A	789	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	734	NAG	1	0
6	A	762	NAG	1	0
6	A	795	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	305/317 (96%)	0.59	42 (13%) 6 6	14, 30, 65, 95	0
2	B	181/184 (98%)	0.56	16 (8%) 15 14	16, 35, 59, 70	0
3	C	214/214 (100%)	0.19	5 (2%) 61 60	12, 27, 53, 64	0
4	D	223/229 (97%)	0.13	13 (5%) 29 27	13, 23, 55, 77	2 (0%)
All	All	923/944 (97%)	0.38	76 (8%) 17 16	12, 29, 59, 95	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	CYS	5.9
1	A	385	CYS	5.2
3	C	2196	CYS	4.7
1	A	410	GLY	4.7
4	D	3148	GLY	4.7
2	B	1141	GLY	4.4
1	A	398	SER	4.1
1	A	231	CYS	4.0
4	D	3001	GLU	4.0
1	A	129	ALA	3.9
1	A	210	PHE	3.8
4	D	3149	GLY	3.8
1	A	228	CYS	3.6
2	B	1130	CYS	3.6
1	A	126	CYS	3.5
1	A	196	CYS	3.4
1	A	267	CYS	3.4
1	A	462	ASN	3.3
1	A	247	CYS	3.3
2	B	1091	GLU	3.2
1	A	445	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	85	VAL	3.1
1	A	84	VAL	3.1
2	B	1181	LYS	3.0
1	A	461	SER	3.0
1	A	125	LEU	2.9
3	C	2001	ASP	2.9
1	A	221	ALA	2.9
2	B	1105	ASP	2.9
4	D	3155	CYS	2.9
1	A	218	CYS	2.8
2	B	1053	ASP	2.7
1	A	99	ASP	2.7
1	A	83	GLU	2.7
1	A	87	VAL	2.7
1	A	128	GLY	2.7
3	C	2214	GLY	2.7
1	A	396	PHE	2.6
1	A	86	LEU	2.6
4	D	3228	PRO	2.6
2	B	1139	GLN	2.5
1	A	119	CYS	2.5
1	A	491	ILE	2.5
1	A	412	ASP	2.5
2	B	1088	ASP	2.5
2	B	1085	GLU	2.5
1	A	194	GLY	2.4
4	D	3205	GLY	2.4
1	A	378	CYS	2.4
2	B	1106	THR	2.4
1	A	463	ASN	2.3
4	D	3110	ASP	2.3
1	A	127	VAL	2.3
1	A	239	CYS	2.3
2	B	1089	GLN	2.3
1	A	418	CYS	2.3
3	C	2154	ASN	2.3
4	D	3229	LYS	2.3
1	A	115	SER	2.2
1	A	350	ARG	2.2
1	A	419	ARG	2.2
2	B	1103	ASN	2.2
4	D	3150	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1180	GLN	2.2
2	B	1104	SER	2.2
4	D	3201	SER	2.2
4	D	3220	THR	2.2
1	A	242	VAL	2.1
4	D	3204	LEU	2.1
4	D	3227	GLU	2.1
1	A	90	THR	2.1
2	B	1122	PRO	2.1
2	B	1001	LYS	2.1
1	A	236	THR	2.0
3	C	2208	THR	2.0
1	A	113	ASP	2.0

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

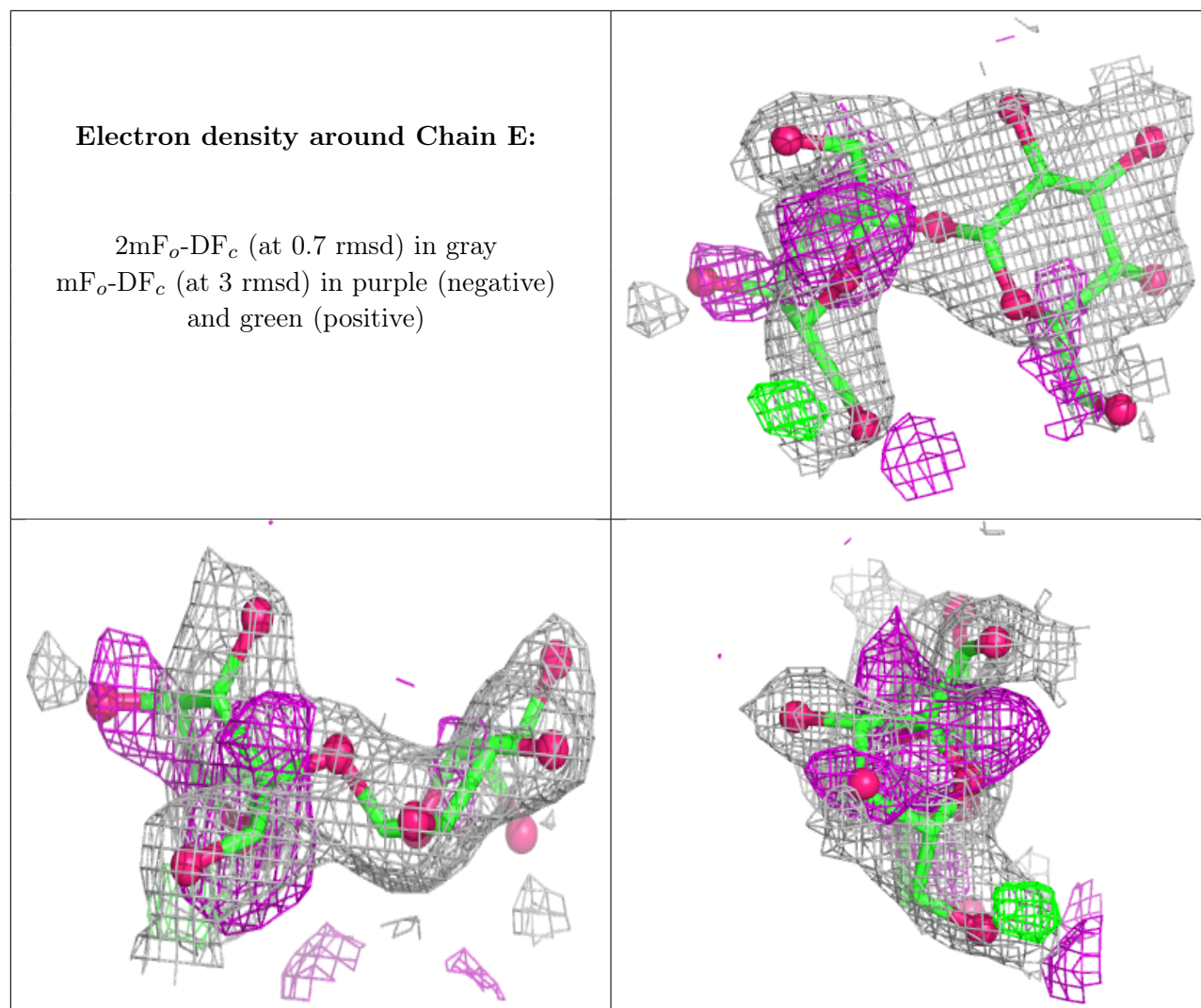
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	FRU	E	2	12/12	0.68	0.20	54,55,55,56	0
5	GLC	E	1	11/12	0.78	0.14	54,54,54,55	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.



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	A	730	14/15	0.38	0.21	54,56,56,57	0
6	NAG	A	697	14/15	0.39	0.19	53,55,55,56	0
6	NAG	A	588	14/15	0.47	0.17	60,61,62,62	0
6	NAG	A	741	14/15	0.48	0.18	52,53,54,54	0
6	NAG	A	839	14/15	0.59	0.16	48,50,51,51	0
6	NAG	A	734	14/15	0.60	0.20	49,50,51,51	0
6	NAG	A	892	14/15	0.64	0.14	42,44,45,45	0
6	NAG	A	948	14/15	0.77	0.13	40,42,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	789	14/15	0.83	0.11	38,39,40,40	0
6	NAG	A	776	14/15	0.83	0.11	36,38,39,39	0
6	NAG	A	795	14/15	0.84	0.13	31,33,34,34	0
6	NAG	A	886	14/15	0.84	0.11	37,38,39,39	0
6	NAG	A	762	14/15	0.85	0.11	28,32,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.