



Full wwPDB X-ray Structure Validation Report i

Jan 15, 2024 – 03:48 pm GMT

PDB ID : 6YA0
Title : Crystal structure of TSWV glycoprotein N ectodomain (Trypsin treated)
Authors : Dessau, M.; Bahat, Y.
Deposited on : 2020-03-11
Resolution : 2.86 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 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 : 1.8.4, 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

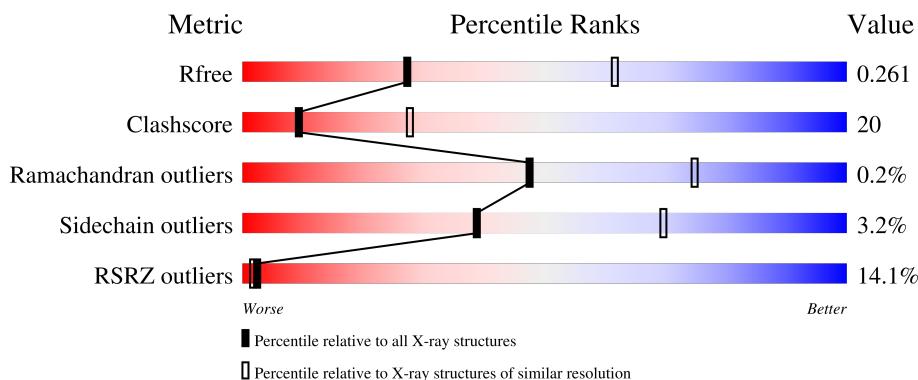
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

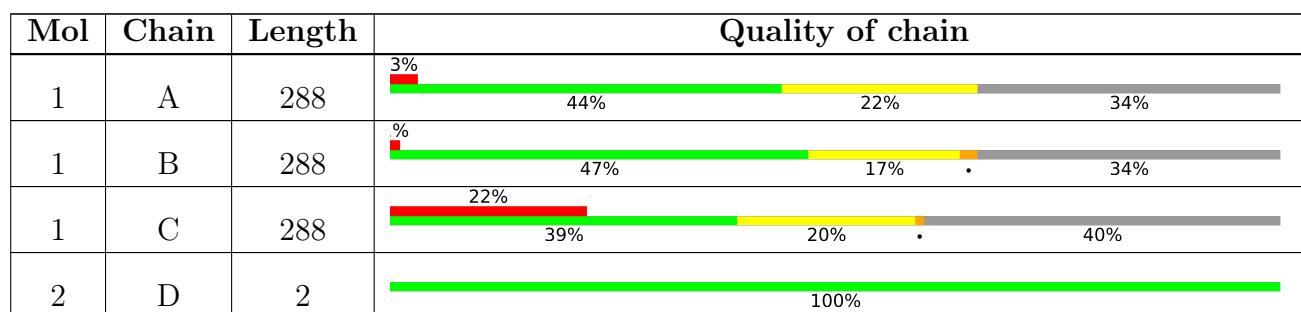
The reported resolution of this entry is 2.86 Å.

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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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.



2 Entry composition [\(i\)](#)

There are 6 unique types of molecules in this entry. The entry contains 4400 atoms, of which 4 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 Glycoprotein.

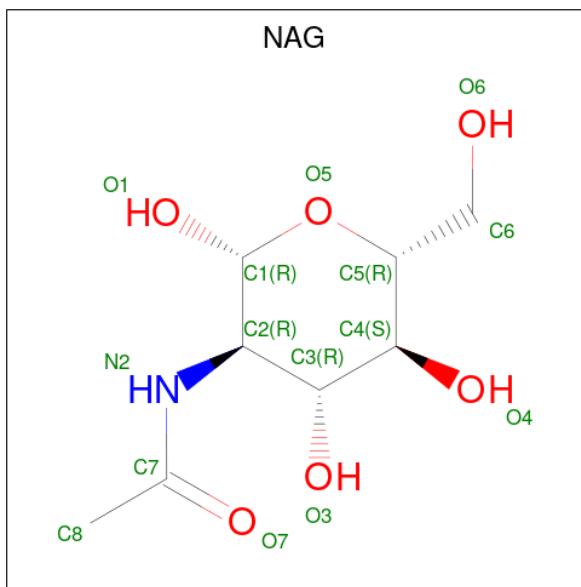
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1467	925	240	294	8			
1	B	189	Total	C	N	O	S	0	0	0
			1460	920	239	293	8			
1	C	174	Total	C	N	O	S	0	0	0
			1337	842	221	266	8			

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



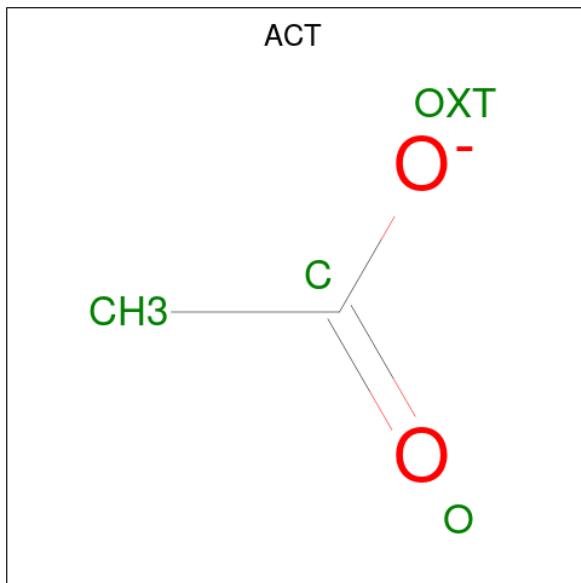
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O		25	0	0
			25	14	1	10				

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



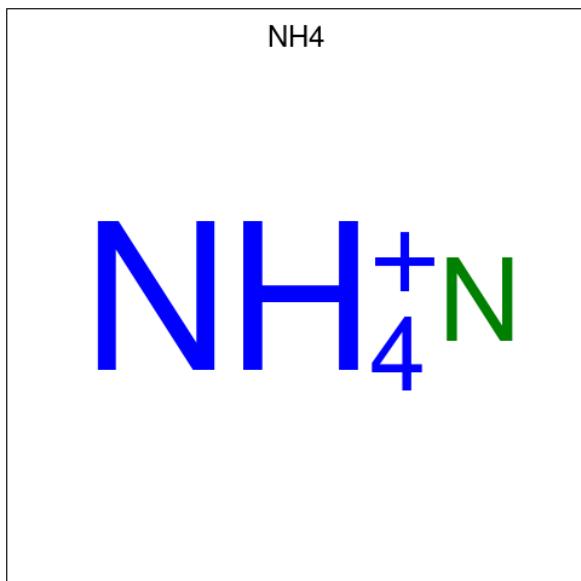
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	14	0
3	A	1	Total C N O 14 8 1 5	14	0
3	B	1	Total C N O 14 8 1 5	14	0
3	B	1	Total C N O 14 8 1 5	14	0
3	C	1	Total C N O 14 8 1 5	14	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2^-$).



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

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total H N 5 4 1	0	0

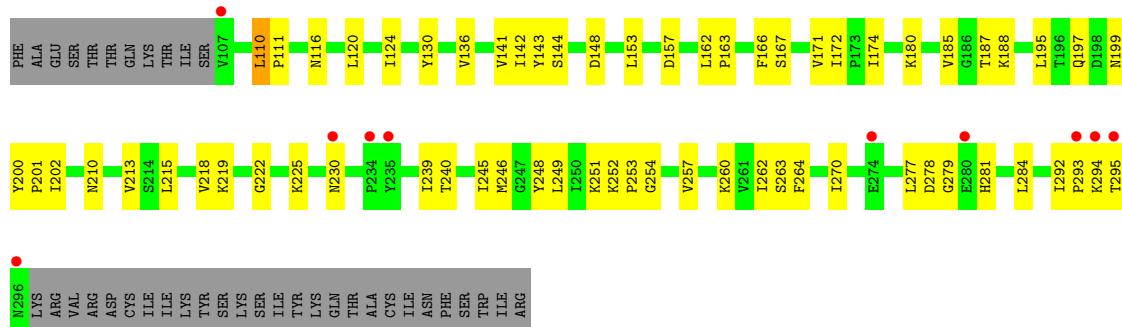
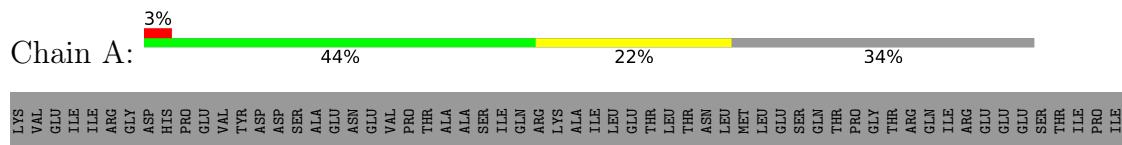
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	B	14	Total O 14 14	0	0
6	C	8	Total O 8 8	0	0

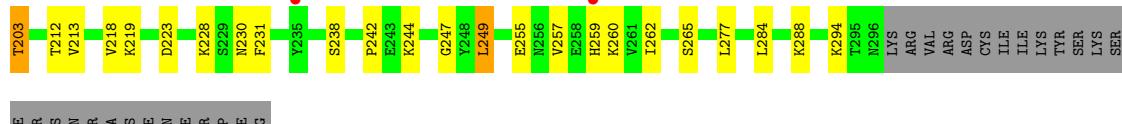
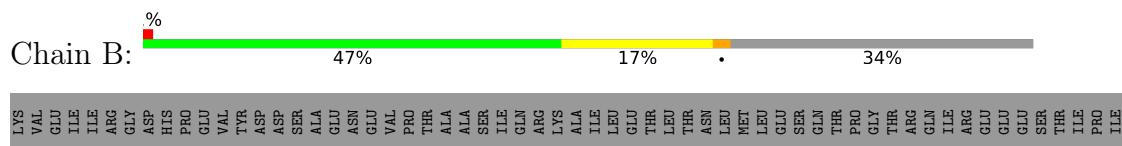
3 Residue-property plots

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.

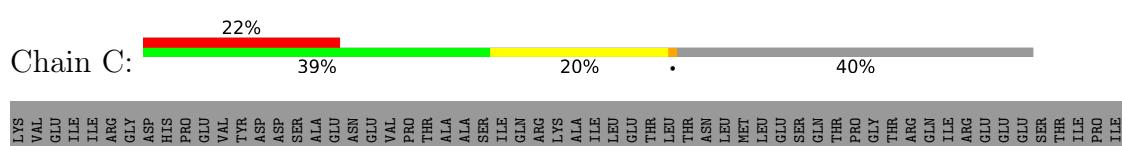
- Molecule 1: Glycoprotein

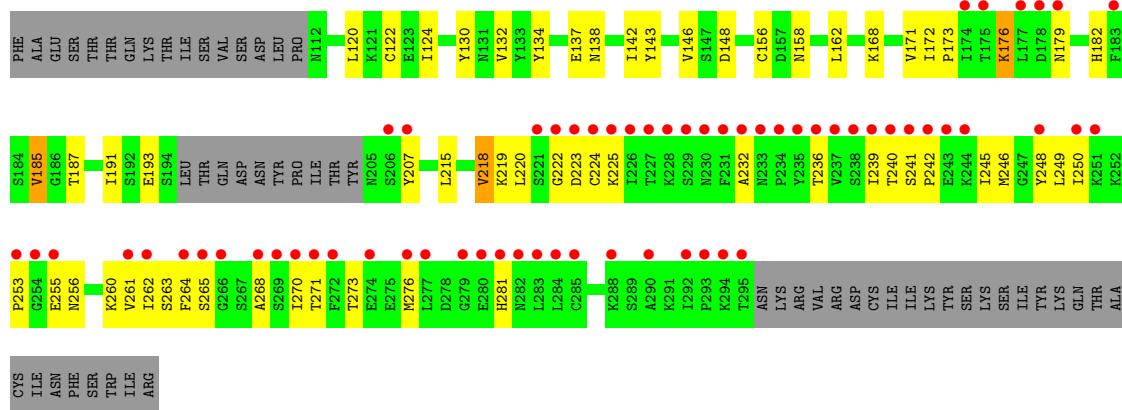


- Molecule 1: Glycoprotein



- Molecule 1: Glycoprotein





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

Chain D:  100%

MAGI
BKA2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.82Å 74.85Å 81.28Å 90.00° 103.27° 90.00°	Depositor
Resolution (Å)	49.91 – 2.86 49.91 – 2.86	Depositor EDS
% Data completeness (in resolution range)	75.9 (49.91-2.86) 76.0 (49.91-2.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.00 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R , R_{free}	0.217 , 0.261 0.217 , 0.261	Depositor DCC
R_{free} test set	1425 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 79.4	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4400	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NH4, ACT

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	0.35	0/1495	0.52	0/2025
1	B	0.34	0/1488	0.53	0/2015
1	C	0.34	0/1360	0.50	0/1835
All	All	0.34	0/4343	0.52	0/5875

There are no bond length outliers.

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	1467	0	1454	51	1
1	B	1460	0	1445	49	1
1	C	1337	0	1332	70	0
2	D	25	0	22	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
4	B	4	0	3	0	0
5	C	1	4	0	0	0
6	A	10	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	0	1	0
6	C	8	0	0	0	0
All	All	4396	4	4321	168	1

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 20.

All (168) 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:249:LEU:HD21	1:C:261:VAL:HA	1.14	1.07
1:B:257:VAL:HG22	1:B:260:LYS:HB3	1.44	0.95
1:B:110:LEU:HG	1:B:143:TYR:HD2	1.32	0.93
1:A:171:VAL:HG22	1:A:218:VAL:HG22	1.52	0.91
1:B:249:LEU:HD11	1:B:257:VAL:HG13	1.52	0.91
1:C:249:LEU:HD11	1:C:261:VAL:HB	1.52	0.89
1:B:257:VAL:HG22	1:B:260:LYS:CB	2.07	0.84
1:C:249:LEU:CD2	1:C:261:VAL:HA	2.04	0.83
1:C:171:VAL:HG12	1:C:218:VAL:HG22	1.61	0.81
1:A:202:ILE:HD13	1:A:213:VAL:HG23	1.62	0.80
1:A:199:ASN:HB3	1:A:210:ASN:O	1.82	0.80
1:B:171:VAL:HG13	1:B:218:VAL:HB	1.64	0.77
1:C:171:VAL:HG11	1:C:218:VAL:CG1	2.15	0.77
1:C:171:VAL:HG11	1:C:218:VAL:HG13	1.68	0.73
1:B:122:CYS:HB3	1:B:136:VAL:HG12	1.71	0.73
1:C:239:ILE:HG22	1:C:264:PHE:CE1	2.25	0.72
1:A:144:SER:HB2	1:A:202:ILE:HG12	1.73	0.70
1:B:249:LEU:HD12	1:B:260:LYS:HG3	1.74	0.69
1:C:185:VAL:HG22	1:C:249:LEU:HD12	1.76	0.68
1:C:250:ILE:HD13	1:C:276:MET:SD	2.35	0.67
1:C:182:HIS:HB3	1:C:253:PRO:HB3	1.77	0.66
1:C:137:GLU:HB2	1:C:142:ILE:HD13	1.80	0.63
1:B:277:LEU:O	1:B:294:LYS:HA	1.97	0.63
1:C:249:LEU:HD21	1:C:261:VAL:CA	2.09	0.62
1:C:124:ILE:HG13	1:C:158:ASN:HB2	1.82	0.62
1:A:279:GLY:N	1:A:294:LYS:HB2	2.14	0.62
1:B:115:LEU:N	1:B:115:LEU:HD22	2.15	0.62
1:C:187:THR:HB	1:C:215:LEU:HD11	1.82	0.62
1:C:273:THR:HB	1:C:276:MET:HB3	1.81	0.62
1:C:225:LYS:HG2	1:C:240:THR:O	2.00	0.61
1:C:249:LEU:HD11	1:C:261:VAL:CB	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLU:H	1:B:154:GLU:CD	2.04	0.59
1:C:122:CYS:HB3	1:C:156:CYS:HA	1.84	0.59
1:A:257:VAL:HG22	1:A:260:LYS:HB2	1.85	0.59
1:A:293:PRO:HB2	1:A:295:THR:CG2	2.33	0.59
1:C:171:VAL:HG12	1:C:218:VAL:CG2	2.33	0.58
1:B:145:CYS:HA	1:B:202:ILE:HG13	1.86	0.58
1:A:153:LEU:HB2	1:A:162:LEU:HD11	1.86	0.58
1:C:171:VAL:CG1	1:C:218:VAL:HG13	2.33	0.58
1:C:171:VAL:HG13	1:C:219:LYS:O	2.04	0.58
1:C:250:ILE:HG23	1:C:281:HIS:HD2	1.69	0.58
1:C:130:TYR:OH	1:C:185:VAL:HG13	2.03	0.58
1:B:108:SER:OG	1:B:109:ASP:N	2.37	0.58
1:C:193:GLU:OE1	1:C:193:GLU:N	2.37	0.58
1:B:171:VAL:CG1	1:B:218:VAL:HB	2.33	0.57
1:C:232:ALA:CB	1:C:236:THR:HB	2.34	0.57
1:A:130:TYR:HB2	1:A:188:LYS:HD2	1.85	0.57
1:B:110:LEU:HG	1:B:143:TYR:CD2	2.24	0.57
1:A:110:LEU:N	1:A:111:PRO:HD2	2.19	0.57
1:C:264:PHE:O	1:C:264:PHE:CG	2.57	0.56
1:C:120:LEU:HD13	1:C:138:ASN:HB2	1.86	0.56
1:C:124:ILE:HA	1:C:134:TYR:HA	1.86	0.56
1:A:195:LEU:HD12	1:A:195:LEU:H	1.71	0.56
1:B:249:LEU:HD12	1:B:260:LYS:CG	2.34	0.56
1:B:257:VAL:HG13	1:B:257:VAL:O	2.05	0.56
1:B:249:LEU:HD11	1:B:257:VAL:CG1	2.33	0.56
1:A:222:GLY:HA3	1:A:246:MET:HE1	1.87	0.56
1:A:249:LEU:HD11	1:A:257:VAL:HG11	1.87	0.55
1:C:262:ILE:H	1:C:262:ILE:HD12	1.70	0.55
1:C:191:ILE:HD11	1:C:207:TYR:CE2	2.42	0.54
1:B:122:CYS:CB	1:B:136:VAL:HG12	2.37	0.54
1:C:171:VAL:CG1	1:C:218:VAL:HG22	2.34	0.54
1:A:200:TYR:CE1	1:A:202:ILE:HD11	2.43	0.54
1:A:225:LYS:HB3	1:A:240:THR:HB	1.90	0.54
1:A:130:TYR:HB3	6:A:501:HOH:O	2.07	0.54
1:A:171:VAL:HG22	1:A:218:VAL:CG2	2.33	0.53
1:A:252:LYS:O	1:A:254:GLY:N	2.42	0.53
1:A:171:VAL:HG23	1:A:219:LYS:O	2.08	0.53
1:C:172:ILE:HG13	1:C:173:PRO:HD2	1.89	0.53
1:A:245:ILE:HD11	1:A:263:SER:HB2	1.91	0.53
1:A:279:GLY:CA	1:A:294:LYS:HB2	2.38	0.53
1:A:174:ILE:HD13	1:A:180:LYS:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ILE:HD13	1:B:127:ILE:HG23	1.90	0.52
1:C:240:THR:HG22	1:C:241:SER:N	2.25	0.52
1:B:128:SER:HB3	1:B:189:PHE:CE2	2.44	0.52
1:B:249:LEU:HD23	1:B:284:LEU:HD12	1.91	0.51
1:A:257:VAL:CG2	1:A:260:LYS:HB2	2.39	0.51
1:B:133:TYR:CE2	1:B:213:VAL:HG11	2.45	0.51
1:B:228:LYS:NZ	6:B:704:HOH:O	2.44	0.51
1:C:239:ILE:HG22	1:C:264:PHE:CZ	2.46	0.51
1:B:171:VAL:HG11	1:B:218:VAL:HG21	1.91	0.51
1:B:260:LYS:HG3	1:B:260:LYS:O	2.11	0.51
1:C:225:LYS:HG2	1:C:240:THR:C	2.31	0.51
1:C:264:PHE:HB2	1:C:268:ALA:HB2	1.92	0.51
1:C:245:ILE:HD11	1:C:263:SER:HB2	1.92	0.51
1:A:116:ASN:O	1:A:120:LEU:HG	2.12	0.50
1:B:150:ALA:HA	1:B:153:LEU:HD12	1.93	0.50
1:C:232:ALA:HB1	1:C:236:THR:HB	1.92	0.50
1:C:245:ILE:HD12	1:C:265:SER:HB3	1.94	0.50
1:C:162:LEU:HD23	1:C:162:LEU:H	1.77	0.49
1:B:141:VAL:HB	1:B:143:TYR:CE1	2.47	0.49
1:A:142:ILE:HD12	1:A:142:ILE:H	1.78	0.49
1:A:249:LEU:HD11	1:A:257:VAL:CG1	2.42	0.49
1:B:110:LEU:N	1:B:111:PRO:HD2	2.27	0.49
1:B:230:ASN:OD1	1:B:230:ASN:N	2.44	0.49
1:A:277:LEU:HA	1:A:292:ILE:HD13	1.95	0.49
1:B:247:GLY:HA2	1:B:262:ILE:O	2.13	0.49
1:C:185:VAL:HG13	1:C:185:VAL:O	2.12	0.48
1:B:111:PRO:O	1:B:115:LEU:HD21	2.14	0.48
1:A:262:ILE:HD12	1:A:262:ILE:N	2.28	0.48
1:A:262:ILE:HD12	1:A:262:ILE:H	1.78	0.47
1:C:225:LYS:HG3	1:C:240:THR:HB	1.96	0.47
1:C:223:ASP:O	1:C:242:PRO:HD2	2.14	0.47
1:A:167:SER:O	6:A:501:HOH:O	2.20	0.47
1:A:171:VAL:CG2	1:A:219:LYS:O	2.63	0.47
1:C:148:ASP:OD1	1:C:168:LYS:HE3	2.15	0.47
1:A:225:LYS:O	1:A:239:ILE:HA	2.14	0.47
1:B:130:TYR:OH	1:B:185:VAL:HG23	2.15	0.47
1:A:278:ASP:OD1	1:A:281:HIS:ND1	2.45	0.46
1:C:236:THR:HA	1:C:270:ILE:O	2.15	0.46
1:A:163:PRO:HG2	1:A:166:PHE:CE1	2.50	0.46
1:C:171:VAL:HG11	1:C:218:VAL:HG11	1.96	0.46
1:C:171:VAL:HG12	1:C:172:ILE:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PRO:HB2	1:A:295:THR:HG23	1.97	0.46
1:C:225:LYS:CG	1:C:240:THR:HB	2.45	0.46
1:B:124:ILE:HA	1:B:134:TYR:CB	2.45	0.46
1:B:128:SER:HB3	1:B:189:PHE:CD2	2.52	0.45
1:B:109:ASP:C	1:B:111:PRO:HD2	2.37	0.45
1:A:144:SER:CB	1:A:202:ILE:HG12	2.46	0.45
1:A:110:LEU:N	1:A:111:PRO:CD	2.80	0.45
1:A:248:TYR:CE1	1:A:270:ILE:HG21	2.51	0.45
1:C:171:VAL:HG22	1:C:220:LEU:HD23	1.98	0.45
1:A:197:GLN:HE21	1:A:197:GLN:HB2	1.67	0.45
1:C:171:VAL:CG1	1:C:218:VAL:CG2	2.94	0.45
1:C:255:GLU:HG3	1:C:256:ASN:H	1.82	0.44
1:A:187:THR:HB	1:A:215:LEU:HD11	1.98	0.44
1:C:250:ILE:HG23	1:C:281:HIS:CD2	2.51	0.44
1:B:192:SER:O	1:B:212:THR:HG22	2.18	0.44
1:C:232:ALA:HB3	1:C:236:THR:HB	2.00	0.44
1:C:236:THR:HG23	1:C:270:ILE:O	2.18	0.43
1:C:176:LYS:HB3	1:C:179:ASN:ND2	2.34	0.43
1:C:264:PHE:O	1:C:264:PHE:CD1	2.71	0.43
1:B:139:ASN:N	1:B:139:ASN:OD1	2.51	0.43
1:C:248:TYR:O	1:C:249:LEU:HD23	2.17	0.43
1:B:131:ASN:HB2	1:B:147:SER:O	2.19	0.43
1:C:222:GLY:HA3	1:C:246:MET:CE	2.49	0.43
1:C:162:LEU:H	1:C:162:LEU:CD2	2.32	0.43
1:A:201:PRO:HA	1:A:210:ASN:HA	2.01	0.43
1:C:222:GLY:HA3	1:C:246:MET:HE1	2.00	0.43
1:B:231:PHE:HB3	1:C:215:LEU:HB2	2.00	0.43
1:A:172:ILE:HD11	1:A:219:LYS:HE3	2.00	0.42
1:A:251:LYS:HD3	1:A:284:LEU:HD11	2.01	0.42
1:C:172:ILE:HG13	1:C:173:PRO:CD	2.48	0.42
1:C:249:LEU:HD23	1:C:249:LEU:HA	1.62	0.42
1:C:249:LEU:HD23	1:C:262:ILE:HD12	2.01	0.42
1:A:174:ILE:HG12	1:A:219:LYS:HB3	2.00	0.42
1:C:120:LEU:CD1	1:C:138:ASN:HB2	2.49	0.42
1:C:191:ILE:HD11	1:C:207:TYR:HE2	1.84	0.42
1:B:145:CYS:HB3	1:B:203:THR:HB	2.02	0.41
1:A:136:VAL:HG22	1:A:143:TYR:HB2	2.02	0.41
1:B:185:VAL:HG23	1:B:185:VAL:O	2.19	0.41
1:C:249:LEU:CD2	1:C:260:LYS:O	2.69	0.41
1:B:142:ILE:HD12	1:B:142:ILE:N	2.35	0.41
1:B:124:ILE:HA	1:B:134:TYR:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ILE:HD11	1:B:219:LYS:HE3	2.02	0.41
1:B:265:SER:HB3	1:C:143:TYR:CE2	2.55	0.41
1:A:148:ASP:O	1:A:166:PHE:HB2	2.20	0.41
1:B:244:LYS:HE2	1:B:244:LYS:HB2	1.87	0.41
1:C:255:GLU:OE2	1:C:255:GLU:HA	2.21	0.41
1:A:230:ASN:O	1:A:230:ASN:ND2	2.53	0.41
1:A:124:ILE:HD11	1:A:153:LEU:HB3	2.02	0.41
1:A:185:VAL:HG22	1:A:219:LYS:HA	2.03	0.41
1:A:239:ILE:HD12	1:A:264:PHE:CE2	2.55	0.41
1:A:252:LYS:O	1:A:252:LYS:HG2	2.20	0.41
1:B:171:VAL:CG1	1:B:218:VAL:CB	2.99	0.40
1:B:110:LEU:N	1:B:111:PRO:CD	2.84	0.40
1:B:223:ASP:O	1:B:242:PRO:HD2	2.21	0.40
1:C:132:VAL:O	1:C:146:VAL:HA	2.22	0.40

All (1) 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:A:157:ASP:OD2	1:B:288:LYS:NZ[2_545]	2.18	0.02

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	188/288 (65%)	175 (93%)	12 (6%)	1 (0%)	29 57
1	B	187/288 (65%)	176 (94%)	11 (6%)	0	100 100
1	C	170/288 (59%)	158 (93%)	12 (7%)	0	100 100
All	All	545/864 (63%)	509 (93%)	35 (6%)	1 (0%)	47 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO

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	174/264 (66%)	172 (99%)	2 (1%)	73 90
1	B	173/264 (66%)	164 (95%)	9 (5%)	23 51
1	C	158/264 (60%)	153 (97%)	5 (3%)	39 69
All	All	505/792 (64%)	489 (97%)	16 (3%)	39 69

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	141	VAL
1	B	124	ILE
1	B	139	ASN
1	B	145	CYS
1	B	193	GLU
1	B	203	THR
1	B	238	SER
1	B	249	LEU
1	B	255	GLU
1	B	259	HIS
1	C	176	LYS
1	C	185	VAL
1	C	218	VAL
1	C	224	CYS
1	C	271	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	GLN
1	A	230	ASN
1	B	113	ASN
1	B	135	GLN
1	C	205	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 [\(i\)](#)

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
2	NAG	D	1	2,1	14,14,15	0.35	0	17,19,21	0.48	0
2	BMA	D	2	2	11,11,12	0.53	0	15,15,17	0.79	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	BMA	D	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

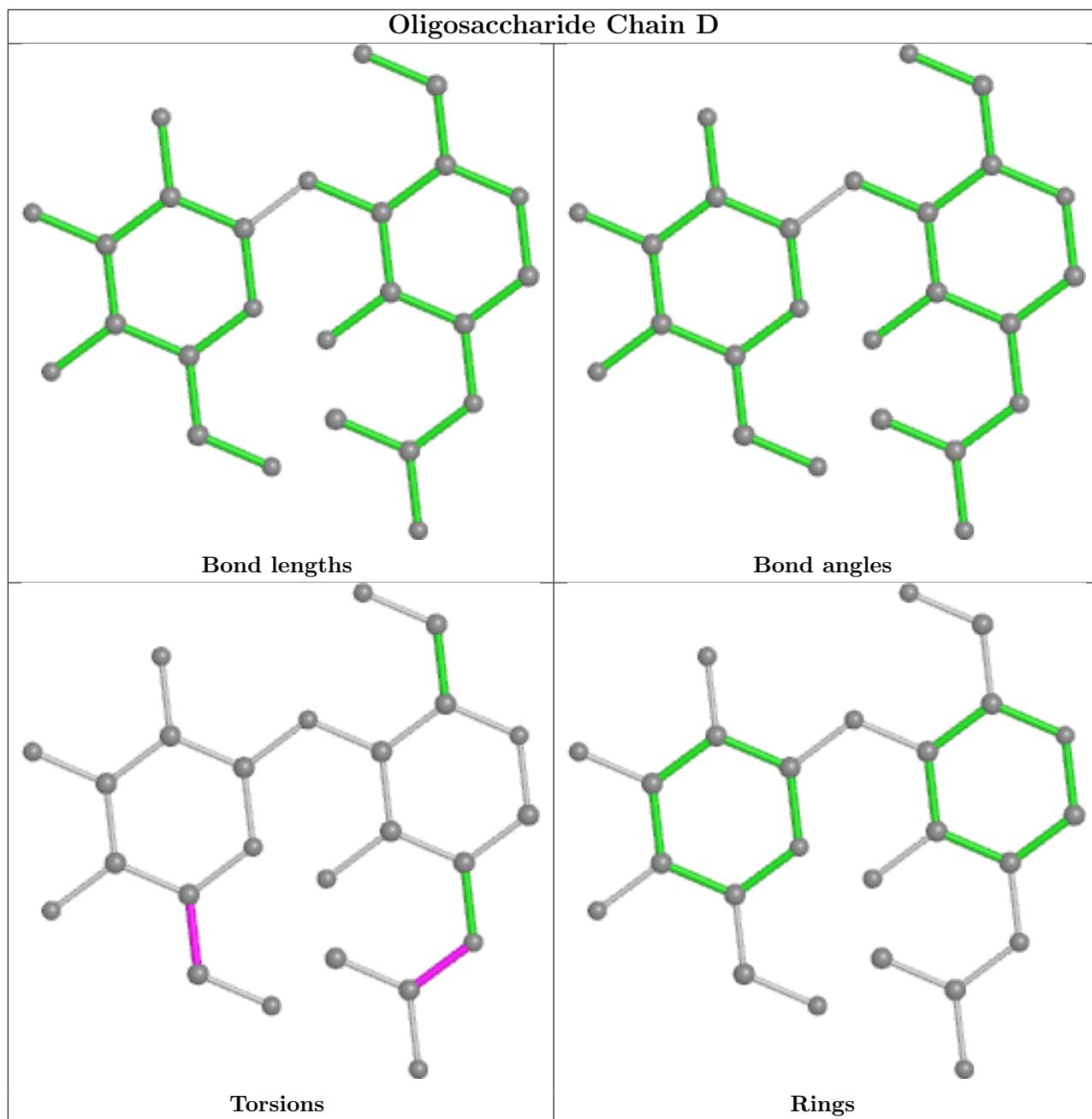
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	BMA	O5-C5-C6-O6

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)

Of 7 ligands modelled in this entry, 1 is modelled with single atom - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	402	1	14,14,15	0.53	0	17,19,21	0.51	0
3	NAG	B	602	1	14,14,15	0.94	2 (14%)	17,19,21	0.72	0
4	ACT	B	601	-	3,3,3	1.31	0	3,3,3	1.50	0
3	NAG	B	603	1	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	C	403	1	14,14,15	0.46	0	17,19,21	0.65	1 (5%)
3	NAG	A	401	1	14,14,15	0.46	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	402	1	-	2/6/23/26	0/1/1/1
3	NAG	B	602	1	-	4/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	C	403	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NAG	O5-C1	-2.39	1.39	1.43
3	B	602	NAG	C1-C2	2.14	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAG	O5-C5-C6-O6
3	A	402	NAG	C4-C5-C6-O6
3	A	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	B	602	NAG	C1-C2-N2-C7
3	B	602	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	602	NAG	C4-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
3	A	401	NAG	C1-C2-N2-C7
3	A	401	NAG	C3-C2-N2-C7
3	C	403	NAG	C3-C2-N2-C7
3	C	403	NAG	C1-C2-N2-C7

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 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	190/288 (65%)	0.40	10 (5%) 26 22	39, 79, 147, 190	0
1	B	189/288 (65%)	0.15	4 (2%) 63 60	30, 64, 113, 147	0
1	C	174/288 (60%)	1.87	64 (36%) 0 0	45, 117, 209, 236	0
All	All	553/864 (64%)	0.78	78 (14%) 2 2	30, 80, 181, 236	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	ILE	9.7
1	C	265	SER	9.5
1	C	235	TYR	9.4
1	C	295	THR	9.2
1	C	266	GLY	7.5
1	A	294	LYS	7.4
1	C	293	PRO	7.1
1	C	279	GLY	7.0
1	C	223	ASP	7.0
1	C	178	ASP	6.8
1	C	227	THR	6.5
1	C	292	ILE	6.5
1	C	237	VAL	6.5
1	C	206	SER	6.3
1	A	235	TYR	6.2
1	C	231	PHE	6.1
1	C	264	PHE	6.0
1	C	238	SER	5.9
1	C	224	CYS	5.9
1	C	236	THR	5.8
1	C	225	LYS	5.4
1	C	272	PHE	5.3
1	C	274	GLU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	239	ILE	5.1
1	C	248	TYR	4.9
1	C	229	SER	4.8
1	A	295	THR	4.8
1	C	290	ALA	4.8
1	C	281	HIS	4.7
1	C	242	PRO	4.5
1	C	280	GLU	4.4
1	C	270	ILE	4.3
1	A	274	GLU	4.1
1	C	234	PRO	4.0
1	C	253	PRO	4.0
1	C	179	ASN	4.0
1	C	230	ASN	4.0
1	C	183	PHE	3.9
1	C	233	ASN	3.9
1	C	294	LYS	3.6
1	C	251	LYS	3.5
1	A	107	VAL	3.4
1	C	228	LYS	3.3
1	C	276	MET	3.2
1	B	111	PRO	3.2
1	C	268	ALA	3.1
1	B	110	LEU	3.1
1	A	296	ASN	3.0
1	C	282	ASN	3.0
1	C	283	LEU	3.0
1	A	234	PRO	2.9
1	C	243	GLU	2.9
1	C	207	TYR	2.9
1	C	221	SER	2.8
1	C	284	LEU	2.8
1	C	241	SER	2.8
1	C	271	THR	2.7
1	B	259	HIS	2.7
1	C	177	LEU	2.7
1	C	254	GLY	2.7
1	C	261	VAL	2.6
1	C	250	ILE	2.6
1	B	235	TYR	2.5
1	A	230	ASN	2.5
1	C	262	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	222	GLY	2.4
1	C	175	THR	2.3
1	C	232	ALA	2.3
1	C	244	LYS	2.3
1	C	255	GLU	2.3
1	A	293	PRO	2.3
1	C	288	LYS	2.2
1	C	240	THR	2.2
1	A	280	GLU	2.2
1	C	285	CYS	2.1
1	C	277	LEU	2.1
1	C	269	SER	2.1
1	C	174	ILE	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [\(i\)](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.