



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 1HWN / pdb_00001hwn
Title : EBULIN COMPLEXED WITH GALACTOSE, TRIGONAL CRYSTAL FORM
Authors : Pascal, J.M.; Day, P.J.; Monzingo, A.F.; Ernst, S.R.; Robertus, J.D.
Deposited on : 2001-01-09
Resolution : 2.80 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

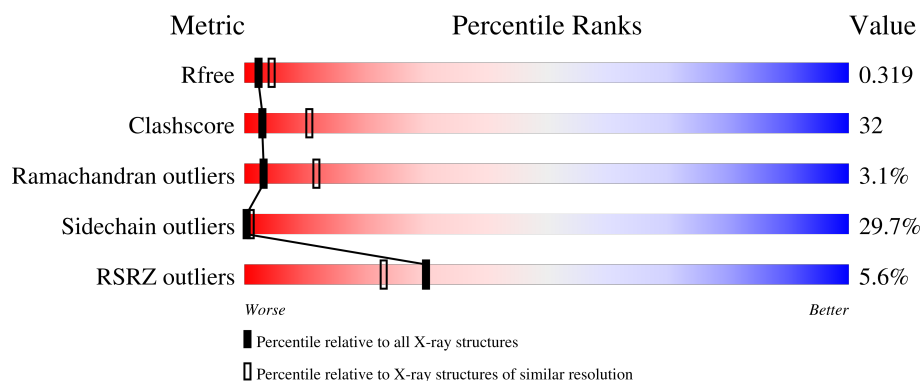
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	254	5% 35% 49% 16%
2	B	266	6% 32% 50% 16% ..
3	C	2	50% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4133 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 EBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2007	1267	344	391	5			

- Molecule 2 is a protein called EBULIN.

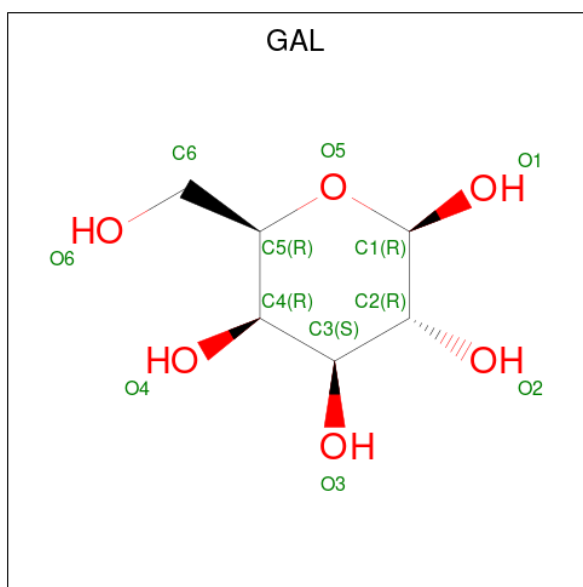
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			2028	1253	359	400	16			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

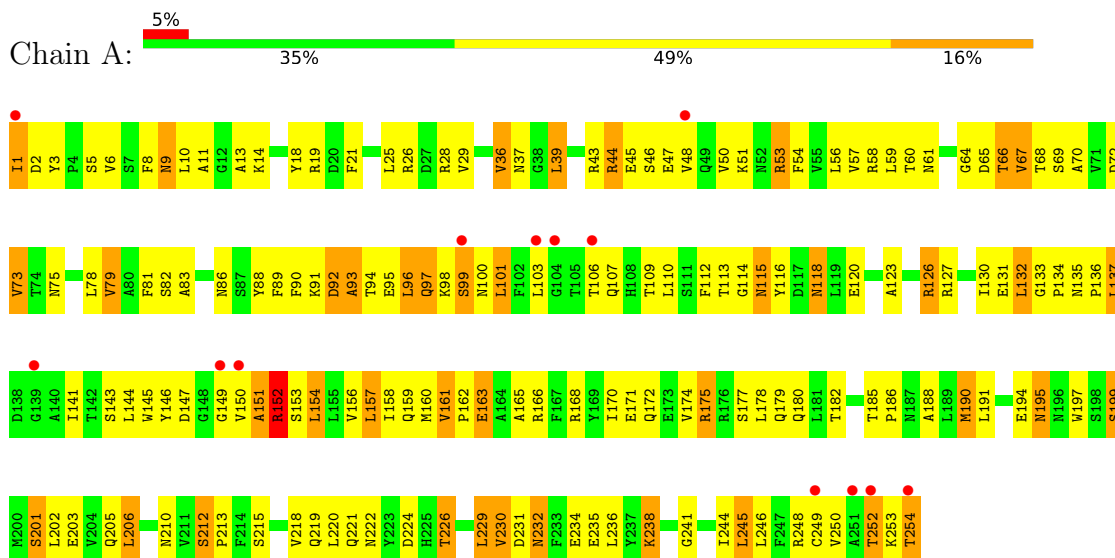
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	27	Total	O	0	0
			27	27		

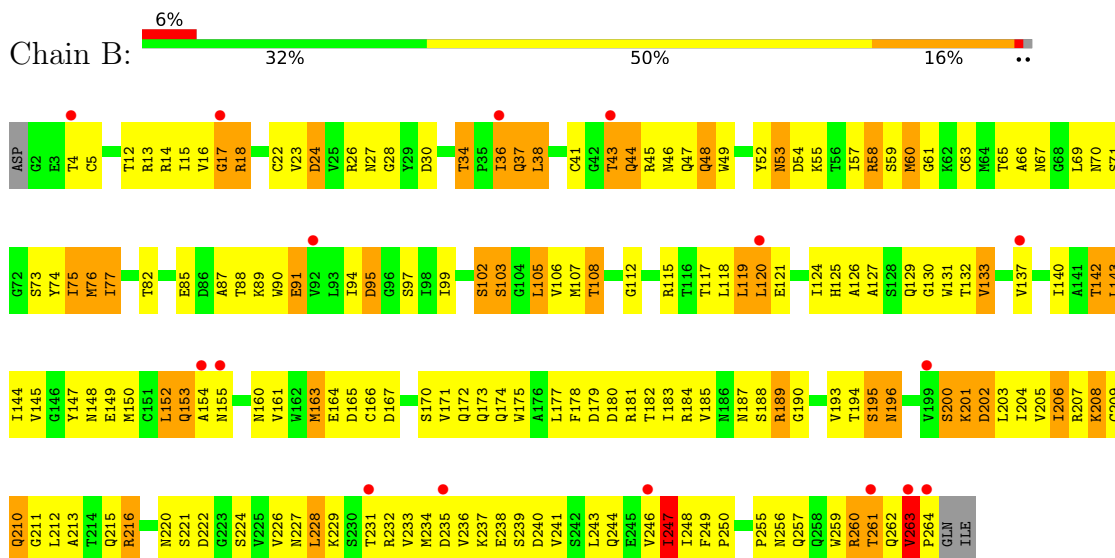
3 Residue-property plots

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.

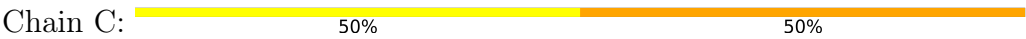
• Molecule 1: EBULIN



• Molecule 2: EBULIN



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.60Å 73.60Å 190.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 93.3 (30.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.264 , 0.328 0.276 , 0.319	Depositor DCC
R_{free} test set	853 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4133	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: GAL, 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	0.28	0/2044	0.68	0/2777
2	B	0.29	0/2065	0.74	1/2813 (0.0%)
All	All	0.29	0/4109	0.71	1/5590 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	247	ILE	N-CA-C	5.22	114.90	108.53

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	2007	0	1982	126	0
2	B	2028	0	1959	144	0
3	C	28	0	25	1	0
4	B	24	0	24	3	0
5	A	19	0	0	0	0
5	B	27	0	0	0	0
All	All	4133	0	3990	259	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 32.

All (259) 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:263:VAL:HB	2:B:264:PRO:HD2	1.44	0.98
2:B:37:GLN:HB3	2:B:117:THR:HA	1.44	0.94
2:B:44:GLN:HG3	2:B:47:GLN:HG3	1.49	0.93
2:B:132:THR:HB	2:B:179:ASP:HB3	1.53	0.87
2:B:177:LEU:HD11	2:B:261:THR:HG21	1.57	0.86
2:B:45:ARG:HA	2:B:48:GLN:HE21	1.38	0.86
2:B:23:VAL:HG22	2:B:36:ILE:HD12	1.60	0.84
2:B:58:ARG:HB3	2:B:63:CYS:HA	1.58	0.84
1:A:127:ARG:HH12	1:A:195:ASN:HD21	1.25	0.82
1:A:134:PRO:HG3	1:A:178:LEU:HA	1.61	0.81
1:A:213:PRO:HG3	2:B:133:VAL:HG11	1.67	0.76
1:A:170:ILE:HG23	1:A:190:MET:HE2	1.69	0.75
2:B:263:VAL:HB	2:B:264:PRO:CD	2.17	0.74
1:A:67:VAL:HG12	1:A:83:ALA:HB2	1.70	0.73
2:B:127:ALA:HB3	2:B:211:GLY:HA2	1.70	0.72
2:B:204:ILE:HD12	2:B:246:VAL:HG12	1.70	0.72
2:B:226:VAL:HG12	2:B:233:VAL:HG13	1.71	0.72
2:B:37:GLN:HA	2:B:118:LEU:HD23	1.71	0.72
2:B:235:ASP:HB3	2:B:257:GLN:HG2	1.73	0.71
2:B:263:VAL:CB	2:B:264:PRO:HD2	2.18	0.70
2:B:200:SER:O	2:B:201:LYS:HB2	1.91	0.69
2:B:124:ILE:H	2:B:129:GLN:HE22	1.41	0.69
1:A:218:VAL:HB	1:A:230:VAL:HG13	1.73	0.69
1:A:202:LEU:O	1:A:206:LEU:HB2	1.92	0.68
2:B:150:MET:HB2	2:B:163:MET:HG2	1.74	0.68
2:B:74:TYR:HA	2:B:119:LEU:HA	1.75	0.68
2:B:85:GLU:HG3	2:B:89:LYS:HE3	1.74	0.68
1:A:45:GLU:HA	1:A:48:VAL:HG12	1.74	0.68
2:B:209:CYS:HA	2:B:215:GLN:HE22	1.57	0.68
1:A:29:VAL:HG12	1:A:73:VAL:HG23	1.77	0.67
2:B:30:ASP:HA	2:B:60:MET:HE3	1.76	0.67
1:A:232:ASN:OD1	1:A:235:GLU:HB2	1.96	0.65
2:B:203:LEU:HA	2:B:247:ILE:HG22	1.77	0.64
1:A:191:LEU:O	1:A:194:GLU:HG2	1.98	0.64
2:B:126:ALA:HA	2:B:213:ALA:HA	1.78	0.64
1:A:61:ASN:OD1	1:A:65:ASP:HB2	1.98	0.63
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD12	1:A:203:GLU:N	2.14	0.63
2:B:108:THR:HG23	2:B:129:GLN:HG2	1.78	0.63
2:B:183:ILE:O	2:B:193:VAL:HG23	1.98	0.63
1:A:115:ASN:OD1	1:A:118:ASN:HB2	1.98	0.63
2:B:256:ASN:HD21	4:B:290:GAL:H2	1.65	0.62
2:B:148:ASN:HB3	2:B:150:MET:HG3	1.82	0.62
2:B:15:ILE:HB	2:B:23:VAL:HG12	1.80	0.62
1:A:161:VAL:HB	1:A:162:PRO:CD	2.30	0.62
2:B:232:ARG:HB3	2:B:248:ILE:HB	1.81	0.61
2:B:154:ALA:HB2	2:B:175:TRP:CH2	2.36	0.61
1:A:154:LEU:HA	1:A:157:LEU:HD12	1.83	0.61
1:A:202:LEU:HD23	1:A:248:ARG:NH1	2.15	0.60
2:B:142:THR:HB	2:B:263:VAL:HA	1.83	0.60
1:A:45:GLU:HA	1:A:48:VAL:CG1	2.31	0.60
2:B:36:ILE:HG22	2:B:118:LEU:HB2	1.83	0.60
1:A:252:THR:HG22	2:B:5:CYS:H	1.67	0.59
1:A:94:THR:O	1:A:97:GLN:HG2	2.02	0.59
2:B:18:ARG:HG2	2:B:112:GLY:HA2	1.85	0.59
2:B:36:ILE:HD11	2:B:49:TRP:HZ2	1.66	0.59
2:B:154:ALA:HB1	2:B:206:ILE:HD13	1.85	0.58
1:A:134:PRO:HG3	1:A:178:LEU:HD23	1.86	0.58
1:A:218:VAL:HB	1:A:230:VAL:CG1	2.33	0.58
1:A:26:ARG:HG3	1:A:165:ALA:HB1	1.86	0.57
1:A:224:ASP:OD1	1:A:226:THR:HB	2.04	0.57
1:A:90:PHE:HB3	1:A:113:THR:HA	1.86	0.57
2:B:45:ARG:HA	2:B:48:GLN:NE2	2.15	0.57
2:B:201:LYS:HA	2:B:247:ILE:HD13	1.86	0.57
1:A:8:PHE:HB2	1:A:21:PHE:CD1	2.39	0.57
1:A:213:PRO:HG3	2:B:133:VAL:CG1	2.33	0.57
1:A:57:VAL:O	1:A:68:THR:HA	2.05	0.57
2:B:161:VAL:HG22	2:B:204:ILE:O	2.05	0.57
1:A:18:TYR:HD2	1:A:175:ARG:HG2	1.71	0.56
1:A:235:GLU:HG2	2:B:140:ILE:HD11	1.87	0.56
1:A:249:CYS:SG	1:A:250:VAL:N	2.78	0.56
1:A:123:ALA:HB2	1:A:151:ALA:HB3	1.87	0.56
2:B:226:VAL:HG12	2:B:233:VAL:HG22	1.86	0.56
1:A:19:ARG:HB2	1:A:175:ARG:CZ	2.36	0.56
1:A:26:ARG:HH21	1:A:165:ALA:HA	1.69	0.56
1:A:10:LEU:HD11	1:A:137:LEU:HD13	1.87	0.56
2:B:209:CYS:C	2:B:210:GLN:HG2	2.31	0.56
2:B:17:GLY:C	2:B:180:ASP:HB3	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:HIS:HB3	2:B:228:LEU:HB3	1.88	0.55
2:B:49:TRP:HB3	2:B:57:ILE:HG22	1.88	0.55
2:B:24:ASP:O	2:B:36:ILE:HD13	2.05	0.55
2:B:166:CYS:HA	2:B:173:GLN:HE22	1.71	0.55
2:B:224:SER:HB2	2:B:233:VAL:HG11	1.89	0.55
1:A:1:ILE:HG12	1:A:100:ASN:HB2	1.88	0.55
1:A:177:SER:HB2	1:A:182:THR:O	2.07	0.55
2:B:23:VAL:O	2:B:23:VAL:HG13	2.08	0.54
2:B:143:LEU:O	2:B:261:THR:HA	2.07	0.54
1:A:199:SER:O	1:A:202:LEU:HG	2.08	0.54
2:B:12:THR:C	2:B:13:ARG:HG2	2.33	0.54
1:A:59:LEU:HD11	1:A:161:VAL:HG21	1.89	0.54
2:B:44:GLN:CG	2:B:47:GLN:HG3	2.33	0.54
1:A:39:LEU:HB2	1:A:245:LEU:HD23	1.90	0.54
2:B:45:ARG:NE	2:B:60:MET:HG3	2.23	0.53
1:A:156:VAL:O	1:A:160:MET:HB2	2.08	0.53
2:B:54:ASP:O	2:B:89:LYS:HD2	2.09	0.52
1:A:97:GLN:O	1:A:101:LEU:HB2	2.09	0.52
1:A:54:PHE:CZ	1:A:97:GLN:HB3	2.44	0.52
1:A:6:VAL:HG21	1:A:25:LEU:HA	1.92	0.52
1:A:201:SER:HA	1:A:245:LEU:HD12	1.91	0.52
2:B:142:THR:HB	2:B:263:VAL:CA	2.39	0.52
1:A:241:GLY:HA3	2:B:260:ARG:HH21	1.74	0.52
2:B:178:PHE:HB3	2:B:180:ASP:OD1	2.09	0.52
1:A:9:ASN:O	1:A:13:ALA:HB2	2.10	0.51
1:A:205:GLN:HE22	1:A:248:ARG:H	1.57	0.51
2:B:17:GLY:O	2:B:18:ARG:HB2	2.10	0.51
1:A:97:GLN:HB2	1:A:101:LEU:HD12	1.92	0.51
1:A:151:ALA:O	1:A:152:ARG:C	2.54	0.51
2:B:91:GLU:HB3	2:B:99:ILE:HG22	1.93	0.51
1:A:172:GLN:HB3	2:B:262:GLN:HE21	1.76	0.51
1:A:91:LYS:HB3	1:A:113:THR:HG22	1.92	0.51
1:A:116:TYR:CD2	1:A:127:ARG:HD3	2.46	0.51
2:B:38:LEU:HD13	2:B:118:LEU:HD21	1.92	0.51
2:B:95:ASP:HB3	2:B:228:LEU:HD11	1.91	0.51
1:A:144:LEU:CD2	1:A:149:GLY:HA2	2.41	0.51
2:B:52:TYR:HB2	2:B:54:ASP:OD1	2.10	0.50
2:B:53:ASN:C	2:B:55:LYS:H	2.20	0.50
2:B:210:GLN:HB2	2:B:212:LEU:HD13	1.92	0.50
2:B:233:VAL:O	2:B:248:ILE:HA	2.11	0.50
2:B:262:GLN:O	2:B:263:VAL:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD12	2:B:5:CYS:SG	2.51	0.50
1:A:53:ARG:HG3	1:A:53:ARG:HH11	1.77	0.50
2:B:167:ASP:H	2:B:173:GLN:NE2	2.10	0.50
2:B:142:THR:HA	2:B:263:VAL:O	2.12	0.49
2:B:194:THR:HB	2:B:207:ARG:HG2	1.93	0.49
2:B:200:SER:O	2:B:201:LYS:CB	2.59	0.49
2:B:34:THR:O	2:B:76:MET:HB2	2.13	0.49
1:A:201:SER:HA	1:A:245:LEU:CD1	2.43	0.49
1:A:48:VAL:HG13	1:A:48:VAL:O	2.12	0.49
2:B:202:ASP:HB2	2:B:248:ILE:HD11	1.93	0.49
1:A:212:SER:HB2	1:A:234:GLU:OE2	2.12	0.49
1:A:53:ARG:NH1	1:A:96:LEU:HD21	2.28	0.49
2:B:127:ALA:HB3	2:B:211:GLY:CA	2.41	0.49
1:A:67:VAL:HG22	1:A:141:ILE:HG23	1.95	0.49
1:A:135:ASN:HB2	1:A:136:PRO:HD3	1.95	0.49
2:B:226:VAL:CG1	2:B:233:VAL:HG22	2.43	0.49
1:A:232:ASN:N	1:A:232:ASN:HD22	2.11	0.48
2:B:188:SER:C	2:B:190:GLY:H	2.20	0.48
1:A:170:ILE:O	1:A:174:VAL:HG23	2.12	0.48
2:B:237:LYS:HG2	2:B:238:GLU:HG2	1.95	0.48
2:B:24:ASP:HB2	2:B:47:GLN:NE2	2.28	0.48
1:A:126:ARG:O	1:A:130:ILE:HD12	2.14	0.48
1:A:110:LEU:HD13	1:A:112:PHE:CZ	2.47	0.48
1:A:100:ASN:HA	1:A:103:LEU:HG	1.95	0.48
1:A:202:LEU:HD23	1:A:248:ARG:CZ	2.44	0.48
1:A:180:GLN:HB2	1:A:182:THR:HG22	1.95	0.48
1:A:249:CYS:SG	2:B:5:CYS:N	2.87	0.48
2:B:30:ASP:HB3	2:B:60:MET:HG2	1.96	0.48
1:A:5:SER:HB3	1:A:56:LEU:HB2	1.95	0.47
1:A:172:GLN:HA	1:A:175:ARG:HB2	1.95	0.47
2:B:180:ASP:O	2:B:181:ARG:HB2	2.13	0.47
1:A:60:THR:HG23	1:A:64:GLY:O	2.15	0.47
2:B:26:ARG:C	2:B:28:GLY:H	2.23	0.47
2:B:153:GLN:HG2	2:B:164:GLU:HB2	1.97	0.47
3:C:2:NAG:O5	3:C:2:NAG:O7	2.33	0.47
2:B:171:VAL:HA	2:B:174:GLN:HG3	1.95	0.47
1:A:53:ARG:HH12	1:A:96:LEU:HD21	1.80	0.47
1:A:252:THR:CG2	2:B:5:CYS:HB2	2.45	0.47
2:B:41:CYS:HB3	2:B:137:VAL:HG11	1.97	0.47
1:A:202:LEU:HD12	1:A:202:LEU:C	2.39	0.46
2:B:59:SER:C	2:B:61:GLY:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB3	1:A:222:ASN:O	2.15	0.46
2:B:263:VAL:O	2:B:264:PRO:C	2.58	0.46
1:A:60:THR:OG1	1:A:66:THR:HB	2.15	0.46
2:B:144:ILE:HG22	2:B:259:TRP:HE3	1.79	0.46
2:B:17:GLY:HA3	2:B:130:GLY:O	2.15	0.46
1:A:114:GLY:O	1:A:115:ASN:HB3	2.15	0.46
1:A:133:GLY:O	1:A:137:LEU:HB2	2.16	0.46
2:B:15:ILE:O	2:B:22:CYS:HA	2.16	0.46
1:A:53:ARG:HH11	1:A:96:LEU:HD11	1.81	0.46
1:A:163:GLU:OE1	1:A:194:GLU:HB2	2.16	0.46
2:B:90:TRP:HH2	2:B:120:LEU:HD21	1.81	0.45
1:A:158:ILE:O	1:A:162:PRO:HG2	2.16	0.45
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.85	0.45
2:B:178:PHE:HB2	2:B:182:THR:O	2.17	0.45
2:B:118:LEU:HD11	2:B:131:TRP:CZ2	2.51	0.45
1:A:92:ASP:O	1:A:93:ALA:C	2.58	0.45
2:B:124:ILE:HG13	2:B:129:GLN:HE22	1.81	0.45
2:B:58:ARG:HB3	2:B:63:CYS:CA	2.40	0.45
1:A:150:VAL:O	1:A:151:ALA:C	2.60	0.44
2:B:49:TRP:HB3	2:B:57:ILE:CG2	2.47	0.44
1:A:195:ASN:HD22	1:A:195:ASN:N	2.15	0.44
2:B:140:ILE:HG22	2:B:142:THR:HG22	1.99	0.44
1:A:10:LEU:HB2	1:A:60:THR:O	2.18	0.44
2:B:99:ILE:HG13	2:B:106:VAL:HG12	1.98	0.44
1:A:238:LYS:HG2	2:B:177:LEU:CD1	2.48	0.44
2:B:226:VAL:CG1	2:B:233:VAL:HG13	2.46	0.44
1:A:144:LEU:HD22	1:A:149:GLY:HA2	2.00	0.44
1:A:230:VAL:HG21	1:A:236:LEU:HB2	1.99	0.44
1:A:232:ASN:N	1:A:232:ASN:ND2	2.66	0.44
2:B:257:GLN:HG3	4:B:290:GAL:O2	2.18	0.44
2:B:220:ASN:HB3	2:B:222:ASP:OD1	2.18	0.43
1:A:98:LYS:H	1:A:98:LYS:HG3	1.64	0.43
1:A:172:GLN:HB3	2:B:262:GLN:NE2	2.32	0.43
2:B:41:CYS:CB	2:B:137:VAL:HG11	2.48	0.43
1:A:166:ARG:HD2	1:A:197:TRP:CE2	2.53	0.43
2:B:144:ILE:HD12	2:B:152:LEU:HD23	2.01	0.43
2:B:260:ARG:NH1	2:B:261:THR:O	2.51	0.43
1:A:229:LEU:HD12	1:A:229:LEU:H	1.83	0.43
2:B:160:ASN:H	2:B:160:ASN:HD22	1.66	0.43
1:A:120:GLU:OE2	1:A:127:ARG:HG3	2.19	0.43
1:A:137:LEU:HB2	1:A:160:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD21	1:A:157:LEU:HD23	2.00	0.43
2:B:43:THR:C	2:B:44:GLN:HG2	2.43	0.43
2:B:238:GLU:C	2:B:240:ASP:H	2.27	0.43
2:B:108:THR:O	2:B:118:LEU:HD13	2.18	0.43
1:A:97:GLN:HB3	1:A:97:GLN:HE21	1.57	0.43
1:A:252:THR:C	1:A:254:THR:H	2.26	0.43
1:A:94:THR:OG1	1:A:96:LEU:HD23	2.19	0.42
1:A:197:TRP:HZ2	1:A:244:ILE:HG22	1.84	0.42
1:A:67:VAL:CG2	1:A:141:ILE:HG23	2.49	0.42
1:A:159:GLN:HA	1:A:163:GLU:HB3	2.01	0.42
2:B:216:ARG:O	2:B:227:ASN:HA	2.19	0.42
2:B:260:ARG:HD3	2:B:262:GLN:HE21	1.84	0.42
1:A:44:ARG:H	1:A:44:ARG:HG3	1.66	0.42
2:B:181:ARG:HA	2:B:181:ARG:HD3	1.78	0.42
1:A:89:PHE:O	1:A:109:THR:HA	2.19	0.42
1:A:197:TRP:CH2	1:A:246:LEU:HB2	2.54	0.42
2:B:235:ASP:CB	2:B:257:GLN:HG2	2.48	0.42
2:B:255:PRO:C	2:B:257:GLN:H	2.28	0.42
2:B:77:ILE:HD13	2:B:77:ILE:H	1.84	0.42
1:A:72:ASP:HB3	1:A:75:ASN:OD1	2.20	0.42
1:A:154:LEU:HA	1:A:154:LEU:HD13	1.87	0.42
2:B:27:ASN:H	4:B:280:GAL:H62	1.85	0.42
1:A:70:ALA:O	1:A:79:VAL:HG12	2.19	0.42
2:B:85:GLU:O	2:B:89:LYS:HG2	2.19	0.42
2:B:108:THR:OG1	2:B:121:GLU:HB2	2.20	0.42
2:B:75:ILE:CD1	2:B:118:LEU:HB3	2.50	0.42
2:B:85:GLU:O	2:B:88:THR:HG22	2.19	0.42
2:B:226:VAL:HG12	2:B:233:VAL:CG1	2.46	0.42
2:B:65:THR:HA	2:B:87:ALA:O	2.20	0.41
1:A:26:ARG:CG	1:A:165:ALA:HB1	2.50	0.41
2:B:126:ALA:HB1	2:B:211:GLY:O	2.19	0.41
2:B:160:ASN:N	2:B:205:VAL:HG12	2.34	0.41
2:B:262:GLN:C	2:B:263:VAL:CG2	2.93	0.41
1:A:37:ASN:OD1	2:B:94:ILE:HG21	2.20	0.41
1:A:168:ARG:O	1:A:171:GLU:HB3	2.20	0.41
2:B:107:MET:CG	2:B:118:LEU:HD12	2.50	0.41
1:A:8:PHE:HB3	1:A:59:LEU:HD23	2.02	0.41
1:A:144:LEU:HD21	1:A:153:SER:HB2	2.03	0.41
1:A:132:LEU:HD11	1:A:186:PRO:HG3	2.03	0.41
2:B:124:ILE:HG13	2:B:129:GLN:NE2	2.35	0.41
2:B:195:SER:OG	2:B:196:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:HB2	1:A:21:PHE:CG	2.55	0.41
1:A:145:TRP:HD1	1:A:146:TYR:HD2	1.69	0.41
1:A:234:GLU:O	1:A:238:LYS:HD3	2.20	0.41
2:B:160:ASN:OD1	2:B:203:LEU:HD13	2.22	0.41
1:A:81:PHE:CE2	1:A:88:TYR:HB2	2.56	0.40
1:A:245:LEU:HD13	1:A:245:LEU:HA	1.88	0.40
2:B:66:ALA:O	2:B:67:ASN:C	2.64	0.40
2:B:14:ARG:O	2:B:133:VAL:HA	2.22	0.40
2:B:126:ALA:O	2:B:216:ARG:NH2	2.54	0.40
1:A:172:GLN:HA	1:A:172:GLN:OE1	2.21	0.40
2:B:240:ASP:OD2	2:B:243:LEU:HG	2.21	0.40
2:B:88:THR:HG23	2:B:89:LYS:HD3	2.04	0.40
2:B:103:SER:O	2:B:105:LEU:HD22	2.21	0.40
2:B:238:GLU:C	2:B:240:ASP:N	2.77	0.40
2:B:249:PHE:CG	2:B:250:PRO:HD2	2.56	0.40
1:A:3:TYR:HE1	1:A:54:PHE:H	1.69	0.40
1:A:99:SER:O	1:A:103:LEU:HD11	2.21	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	252/254 (99%)	218 (86%)	27 (11%)	7 (3%)	4	14
2	B	261/266 (98%)	212 (81%)	40 (15%)	9 (3%)	3	11
All	All	513/520 (99%)	430 (84%)	67 (13%)	16 (3%)	3	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	187	ASN

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Mol	Chain	Res	Type
2	B	263	VAL
1	A	11	ALA
1	A	93	ALA
1	A	115	ASN
1	A	151	ALA
2	B	18	ARG
2	B	69	LEU
1	A	161	VAL
2	B	102	SER
2	B	189	ARG
2	B	201	LYS
1	A	152	ARG
2	B	208	LYS
1	A	36	VAL
2	B	17	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/223 (100%)	157 (70%)	66 (30%)	0	1
2	B	228/231 (99%)	160 (70%)	68 (30%)	0	1
All	All	451/454 (99%)	317 (70%)	134 (30%)	0	1

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	2	ASP
1	A	9	ASN
1	A	14	LYS
1	A	28	ARG
1	A	36	VAL
1	A	39	LEU
1	A	43	ARG

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Mol	Chain	Res	Type
1	A	44	ARG
1	A	46	SER
1	A	47	GLU
1	A	50	VAL
1	A	51	LYS
1	A	53	ARG
1	A	58	ARG
1	A	66	THR
1	A	67	VAL
1	A	69	SER
1	A	73	VAL
1	A	78	LEU
1	A	79	VAL
1	A	82	SER
1	A	86	ASN
1	A	92	ASP
1	A	95	GLU
1	A	96	LEU
1	A	97	GLN
1	A	99	SER
1	A	101	LEU
1	A	106	THR
1	A	107	GLN
1	A	118	ASN
1	A	126	ARG
1	A	131	GLU
1	A	132	LEU
1	A	137	LEU
1	A	143	SER
1	A	147	ASP
1	A	152	ARG
1	A	154	LEU
1	A	157	LEU
1	A	163	GLU
1	A	175	ARG
1	A	179	GLN
1	A	185	THR
1	A	190	MET
1	A	195	ASN
1	A	199	SER
1	A	201	SER
1	A	206	LEU

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	212	SER
1	A	215	SER
1	A	219	GLN
1	A	220	LEU
1	A	221	GLN
1	A	226	THR
1	A	229	LEU
1	A	230	VAL
1	A	231	ASP
1	A	232	ASN
1	A	238	LYS
1	A	245	LEU
1	A	252	THR
1	A	253	LYS
1	A	254	THR
2	B	4	THR
2	B	16	VAL
2	B	24	ASP
2	B	34	THR
2	B	36	ILE
2	B	37	GLN
2	B	38	LEU
2	B	43	THR
2	B	44	GLN
2	B	46	ASN
2	B	48	GLN
2	B	53	ASN
2	B	58	ARG
2	B	60	MET
2	B	70	ASN
2	B	71	SER
2	B	73	SER
2	B	75	ILE
2	B	76	MET
2	B	77	ILE
2	B	82	THR
2	B	91	GLU
2	B	95	ASP
2	B	97	SER
2	B	102	SER
2	B	103	SER

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Mol	Chain	Res	Type
2	B	105	LEU
2	B	108	THR
2	B	115	ARG
2	B	119	LEU
2	B	120	LEU
2	B	133	VAL
2	B	142	THR
2	B	143	LEU
2	B	145	VAL
2	B	147	TYR
2	B	149	GLU
2	B	152	LEU
2	B	153	GLN
2	B	155	ASN
2	B	163	MET
2	B	165	ASP
2	B	170	SER
2	B	172	GLN
2	B	184	ARG
2	B	185	VAL
2	B	189	ARG
2	B	195	SER
2	B	196	ASN
2	B	200	SER
2	B	202	ASP
2	B	206	ILE
2	B	208	LYS
2	B	210	GLN
2	B	216	ARG
2	B	221	SER
2	B	228	LEU
2	B	229	LYS
2	B	231	THR
2	B	234	MET
2	B	236	VAL
2	B	239	SER
2	B	241	VAL
2	B	244	GLN
2	B	247	ILE
2	B	260	ARG
2	B	261	THR
2	B	263	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	118	ASN
1	A	135	ASN
1	A	172	GLN
1	A	195	ASN
1	A	205	GLN
1	A	221	GLN
2	B	27	ASN
2	B	48	GLN
2	B	70	ASN
2	B	129	GLN
2	B	159	ASN
2	B	173	GLN
2	B	210	GLN
2	B	215	GLN
2	B	244	GLN
2	B	256	ASN
2	B	262	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
3	NAG	C	1	3,2	14,14,15	0.46	0	17,19,21	0.66	1 (5%)
3	NAG	C	2	3	14,14,15	0.63	0	17,19,21	1.17	2 (11%)

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	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	2.46	115.48	112.19
3	C	2	NAG	C3-C4-C5	2.06	113.97	110.23
3	C	1	NAG	C2-N2-C7	-2.05	120.16	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

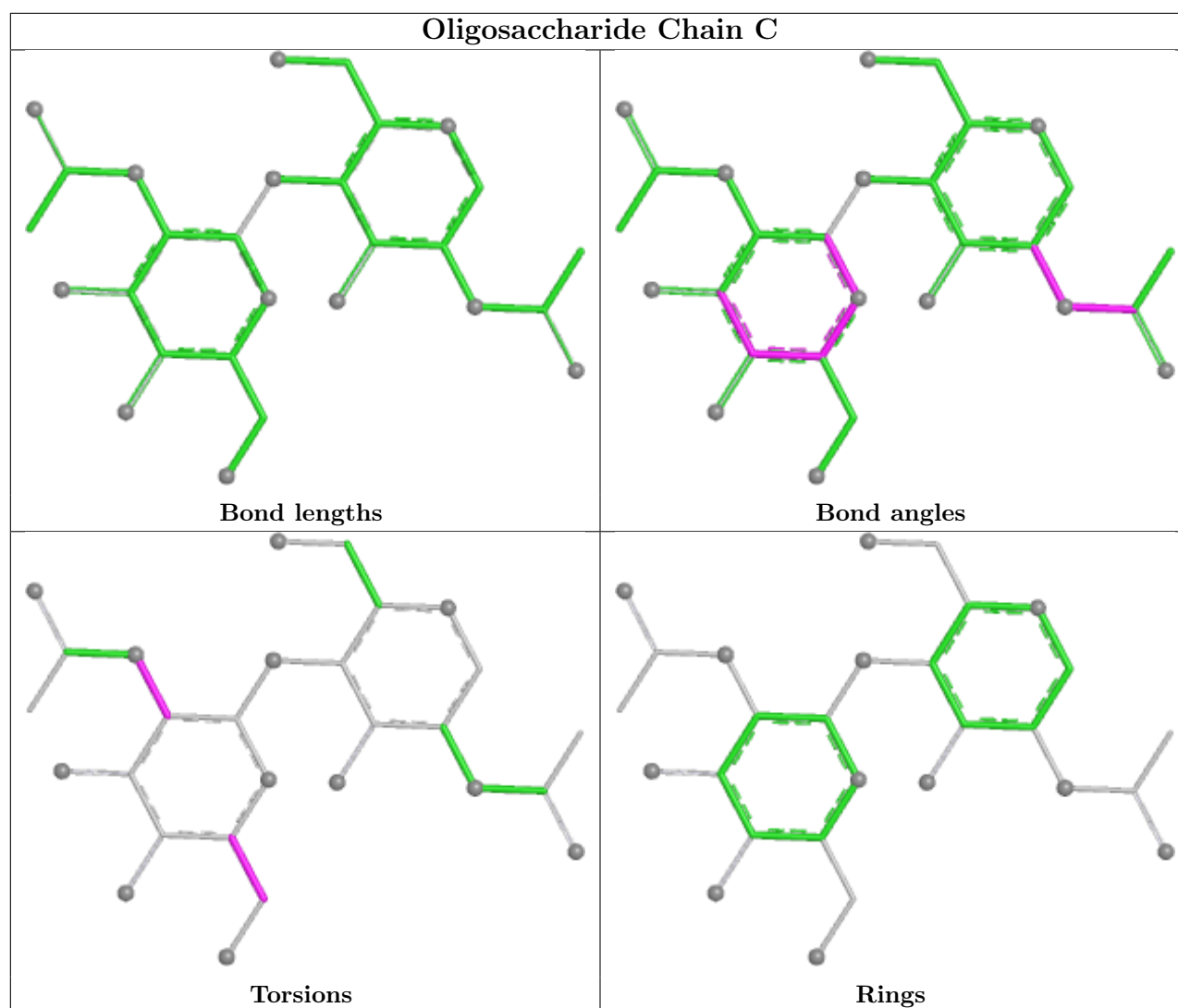
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C1-C2-N2-C7
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	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](#)

2 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	GAL	B	290	-	12,12,12	0.33	0	17,17,17	0.36	0
4	GAL	B	280	-	12,12,12	0.33	0	17,17,17	0.34	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	GAL	B	290	-	-	0/2/22/22	0/1/1/1
4	GAL	B	280	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	280	GAL	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	290	GAL	2	0
4	B	280	GAL	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	254/254 (100%)	0.75	13 (5%) 33 25	7, 26, 48, 60	0
2	B	263/266 (98%)	0.85	16 (6%) 27 20	4, 29, 46, 63	0
All	All	517/520 (99%)	0.80	29 (5%) 30 23	4, 28, 47, 63	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	264	PRO	4.4
1	A	150	VAL	3.8
1	A	252	THR	3.4
2	B	263	VAL	3.3
1	A	1	ILE	3.0
2	B	231	THR	2.9
1	A	254	THR	2.9
1	A	106	THR	2.9
2	B	199	VAL	2.8
2	B	36	ILE	2.8
2	B	17	GLY	2.8
2	B	154	ALA	2.6
2	B	4	THR	2.6
1	A	104	GLY	2.5
2	B	43	THR	2.5
2	B	246	VAL	2.4
1	A	249	CYS	2.4
2	B	137	VAL	2.4
2	B	261	THR	2.4
2	B	120	LEU	2.3
2	B	92	VAL	2.3
1	A	103	LEU	2.3
1	A	48	VAL	2.2
1	A	99	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	2.2
2	B	155	ASN	2.2
2	B	235	ASP	2.2
1	A	139	GLY	2.1
1	A	251	ALA	2.1

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

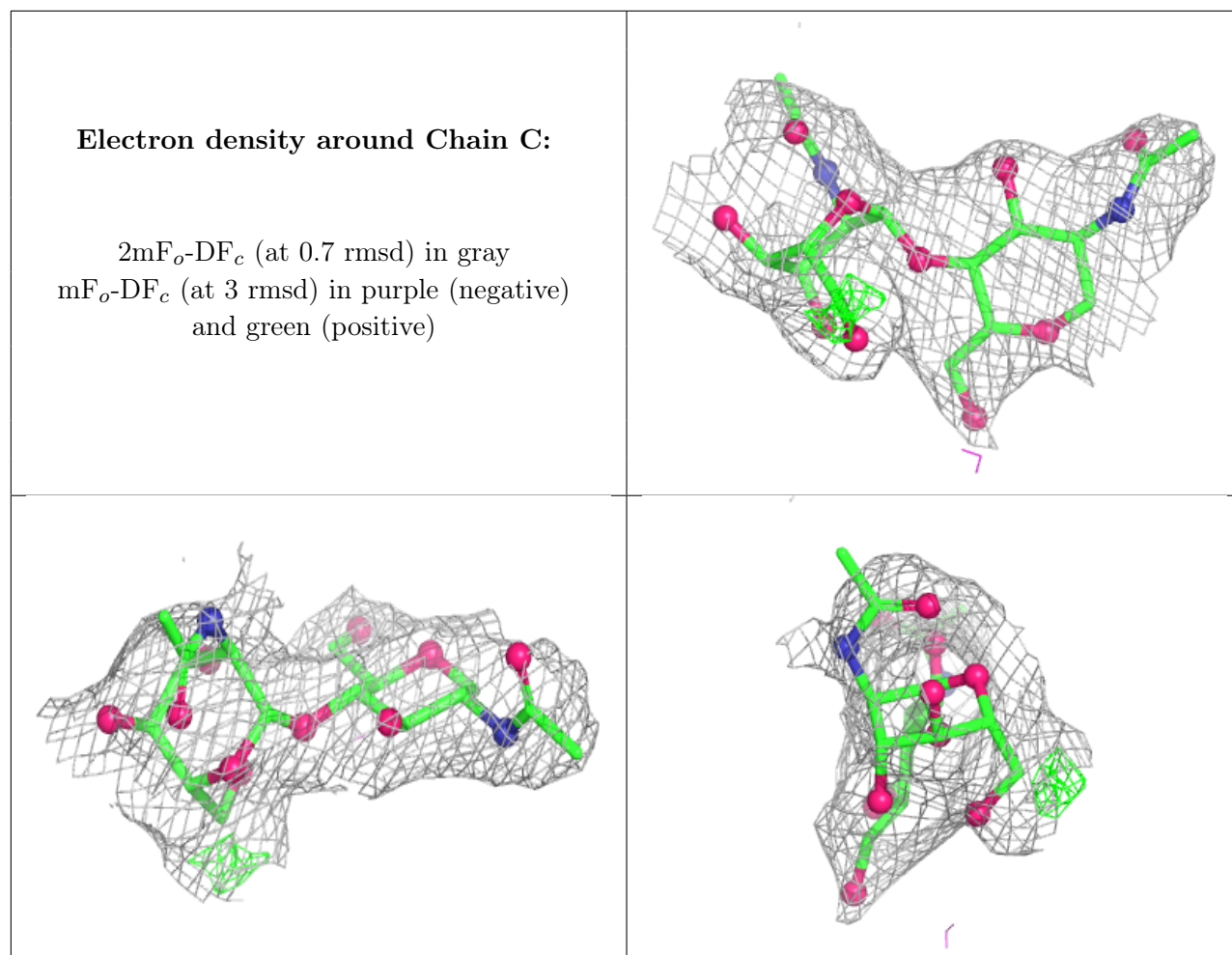
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	C	2	14/15	0.57	0.17	68,68,68,68	0
3	NAG	C	1	14/15	0.81	0.13	30,30,30,30	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($\text{\AA}^2$)	Q<0.9
4	GAL	B	290	12/12	0.57	0.20	51,51,51,51	0
4	GAL	B	280	12/12	0.72	0.20	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.