



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:26 AM UTC

PDB ID : 7ODU / pdb_00007odu
Title : Natural killer cell receptor NKR-P1B from *Rattus norvegicus* in complex with its cognate ligand Clr-11
Authors : Skalova, T.; Blaha, J.; Kalouskova, B.; Skorepa, O.; Vanek, O.; Dohnalek, J.
Deposited on : 2021-04-30
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

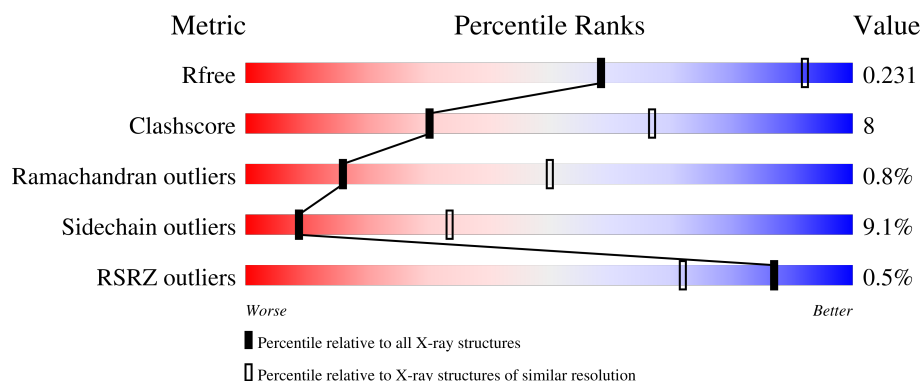
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	133	2% 74% 18% 5% .
1	B	133	71% 17% . 8%
2	C	151	54% 23% . 20%
3	D	2	100%
3	E	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3154 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 C-type lectin domain family 2 member D11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1080	685	192	199	4			
1	B	122	Total	C	N	O	S	0	0	0
			1019	649	175	191	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ILE	-	expression tag	UNP Q0H8B9
A	75	THR	-	expression tag	UNP Q0H8B9
A	76	GLY	-	expression tag	UNP Q0H8B9
A	192	ARG	LYS	variant	UNP Q0H8B9
A	196	GLY	-	expression tag	UNP Q0H8B9
A	197	THR	-	expression tag	UNP Q0H8B9
A	198	HIS	-	expression tag	UNP Q0H8B9
A	199	HIS	-	expression tag	UNP Q0H8B9
A	200	HIS	-	expression tag	UNP Q0H8B9
A	201	HIS	-	expression tag	UNP Q0H8B9
A	202	HIS	-	expression tag	UNP Q0H8B9
A	203	HIS	-	expression tag	UNP Q0H8B9
A	204	HIS	-	expression tag	UNP Q0H8B9
A	205	HIS	-	expression tag	UNP Q0H8B9
A	206	GLY	-	expression tag	UNP Q0H8B9
B	74	ILE	-	expression tag	UNP Q0H8B9
B	75	THR	-	expression tag	UNP Q0H8B9
B	76	GLY	-	expression tag	UNP Q0H8B9
B	192	ARG	LYS	variant	UNP Q0H8B9
B	196	GLY	-	expression tag	UNP Q0H8B9
B	197	THR	-	expression tag	UNP Q0H8B9
B	198	HIS	-	expression tag	UNP Q0H8B9
B	199	HIS	-	expression tag	UNP Q0H8B9
B	200	HIS	-	expression tag	UNP Q0H8B9
B	201	HIS	-	expression tag	UNP Q0H8B9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	202	HIS	-	expression tag	UNP Q0H8B9
B	203	HIS	-	expression tag	UNP Q0H8B9
B	204	HIS	-	expression tag	UNP Q0H8B9
B	205	HIS	-	expression tag	UNP Q0H8B9
B	206	GLY	-	expression tag	UNP Q0H8B9

- Molecule 2 is a protein called Killer cell lectin-like receptor subfamily B member 1B allele A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	121	Total	C	N	O	S	0	0	0
			956	594	164	192	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	75	GLY	-	expression tag	UNP A4KWA1
C	76	THR	-	expression tag	UNP A4KWA1
C	77	GLY	-	expression tag	UNP A4KWA1
C	224	GLY	-	expression tag	UNP A4KWA1
C	225	THR	-	expression tag	UNP A4KWA1

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

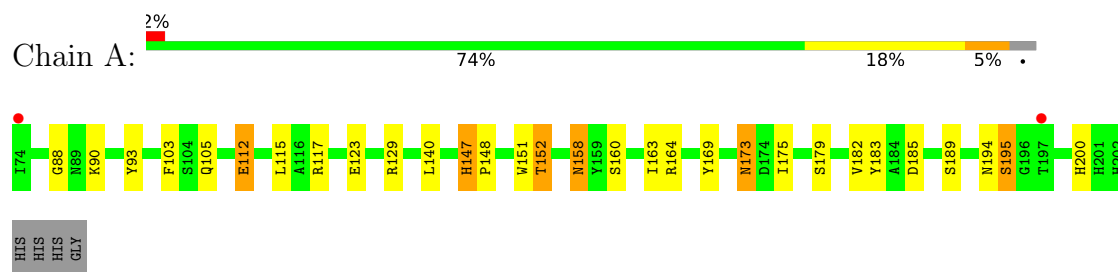
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

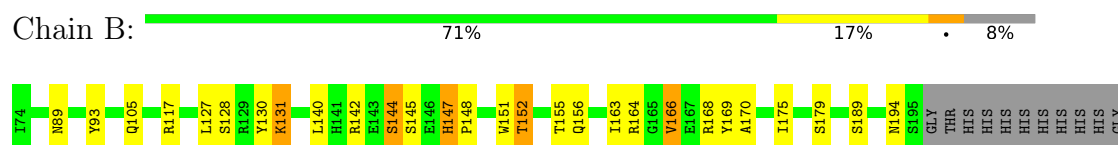
3 Residue-property plots [i](#)

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.

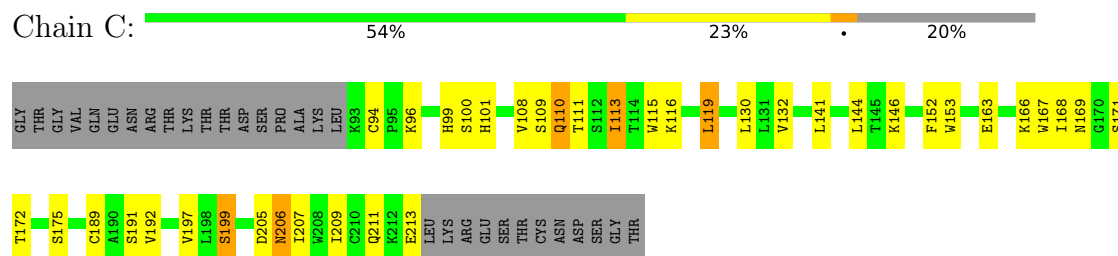
- Molecule 1: C-type lectin domain family 2 member D11



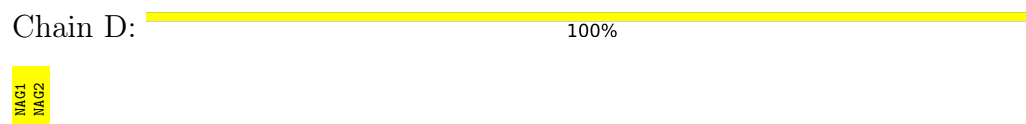
- Molecule 1: C-type lectin domain family 2 member D11



- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele A



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



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

Chain E:



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.59Å 111.59Å 110.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 3.00 49.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.77-3.00) 99.9 (49.77-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.259 0.211 , 0.231	Depositor DCC
R_{free} test set	783 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	94.5	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3154	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: NAG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	0/1117	1.41	4/1514 (0.3%)
1	B	0.98	0/1051	1.41	2/1424 (0.1%)
2	C	1.09	0/975	1.54	7/1317 (0.5%)
All	All	1.04	0/3143	1.45	13/4255 (0.3%)

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	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASN	CB-CA-C	7.29	122.39	111.17
2	C	109	SER	O-C-N	5.77	129.93	122.89
2	C	109	SER	N-CA-CB	5.73	118.39	109.97
2	C	109	SER	CA-C-N	5.52	130.36	122.08
2	C	109	SER	C-N-CA	5.52	130.36	122.08
2	C	199	SER	CA-C-O	-5.46	114.74	120.58
2	C	119	LEU	CA-C-N	5.41	127.97	120.29
2	C	119	LEU	C-N-CA	5.41	127.97	120.29
1	A	185	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	144	SER	CA-C-N	5.11	127.84	120.38
1	B	144	SER	C-N-CA	5.11	127.84	120.38
1	A	195	SER	CA-C-N	5.09	126.76	120.34
1	A	195	SER	C-N-CA	5.09	126.76	120.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1080	0	975	22	0
1	B	1019	0	931	17	0
2	C	956	0	912	18	0
3	D	28	0	25	0	0
3	E	28	0	25	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
5	A	1	0	0	0	0
All	All	3154	0	2907	51	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 8.

All (51) 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:C:94:CYS:SG	2:C:100:SER:HB3	2.24	0.77
1:A:169:TYR:CE1	1:A:182:VAL:HG23	2.21	0.76
1:A:173:ASN:HD21	2:C:205:ASP:HB2	1.53	0.73
1:A:105:GLN:OE1	1:A:152:THR:HG22	1.96	0.66
1:A:173:ASN:HB3	1:A:175:ILE:H	1.62	0.64
1:A:140:LEU:HD13	1:A:163:ILE:HD11	1.81	0.62
1:A:129:ARG:HD3	1:B:130:TYR:CE1	2.36	0.59
1:A:129:ARG:HD3	1:B:130:TYR:CZ	2.38	0.59
1:A:183:TYR:OH	2:C:199:SER:O	2.19	0.59
1:A:169:TYR:CE1	1:A:182:VAL:CG2	2.86	0.58
2:C:192:VAL:HG22	2:C:197:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:PHE:CD1	2:C:209:ILE:HD12	2.40	0.57
2:C:152:PHE:O	2:C:191:SER:HA	2.03	0.57
1:B:140:LEU:HD13	1:B:163:ILE:HD11	1.87	0.57
1:B:89:ASN:O	1:B:194:ASN:ND2	2.37	0.56
1:B:142:ARG:O	1:B:168:ARG:HG3	2.06	0.55
1:A:112:GLU:OE1	1:A:200:HIS:HA	2.07	0.55
1:A:173:ASN:ND2	2:C:205:ASP:HB2	2.21	0.55
1:B:166:VAL:HG22	1:B:166:VAL:O	2.07	0.55
1:A:117:ARG:HA	1:A:151:TRP:CZ3	2.46	0.49
1:B:105:GLN:OE1	1:B:152:THR:HG22	2.12	0.49
2:C:167:TRP:C	2:C:169:ASN:H	2.20	0.49
2:C:99:HIS:ND1	2:C:144:LEU:HD11	2.28	0.48
1:B:117:ARG:HA	1:B:151:TRP:CZ3	2.48	0.48
2:C:153:TRP:CE2	2:C:206:ASN:HB2	2.49	0.48
2:C:113:ILE:O	2:C:205:ASP:HA	2.15	0.47
1:A:169:TYR:CZ	1:A:182:VAL:CG2	2.99	0.45
1:B:127:LEU:O	1:B:131:LYS:HB2	2.17	0.45
1:B:144:SER:OG	1:B:145:SER:N	2.50	0.45
1:A:164:ARG:NH2	2:C:205:ASP:OD2	2.34	0.44
2:C:115:TRP:CG	2:C:189:CYS:SG	3.11	0.44
1:B:166:VAL:O	1:B:166:VAL:CG2	2.66	0.44
1:B:169:TYR:O	1:B:179:SER:HA	2.18	0.44
1:A:147:HIS:N	1:A:147:HIS:ND1	2.66	0.44
1:B:93:TYR:O	1:B:189:SER:HA	2.18	0.43
1:A:93:TYR:O	1:A:189:SER:HA	2.18	0.43
2:C:130:LEU:CD2	2:C:132:VAL:HG22	2.50	0.42
2:C:132:VAL:O	3:E:2:NAG:H82	2.20	0.42
1:B:140:LEU:HB2	1:B:170:ALA:HB3	2.01	0.42
1:B:147:HIS:N	1:B:147:HIS:ND1	2.67	0.42
1:A:169:TYR:O	1:A:179:SER:HA	2.19	0.42
1:A:88:GLY:C	1:A:90:LYS:H	2.28	0.41
1:A:103:PHE:CD1	1:A:103:PHE:C	2.98	0.41
1:B:155:THR:HG22	1:B:156:GLN:O	2.20	0.41
1:B:147:HIS:HB3	1:B:148:PRO:CD	2.50	0.41
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.98	0.41
2:C:115:TRP:CD1	2:C:189:CYS:HB3	2.56	0.41
1:A:147:HIS:HB3	1:A:148:PRO:CD	2.51	0.40
2:C:110:GLN:O	2:C:110:GLN:CG	2.69	0.40
1:A:90:LYS:HE3	1:A:123:GLU:OE1	2.22	0.40
2:C:130:LEU:HD13	2:C:141:LEU:HD11	2.03	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	127/133 (96%)	109 (86%)	17 (13%)	1 (1%)	16	50
1	B	120/133 (90%)	107 (89%)	12 (10%)	1 (1%)	16	50
2	C	119/151 (79%)	103 (87%)	15 (13%)	1 (1%)	16	50
All	All	366/417 (88%)	319 (87%)	44 (12%)	3 (1%)	16	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	B	131	LYS
2	C	168	ILE

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	112/115 (97%)	106 (95%)	6 (5%)	20	53
1	B	106/115 (92%)	100 (94%)	6 (6%)	18	52
2	C	110/136 (81%)	92 (84%)	18 (16%)	2	12
All	All	328/366 (90%)	298 (91%)	30 (9%)	9	33

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	147	HIS
1	A	152	THR
1	A	158	ASN
1	A	173	ASN
1	A	194	ASN
1	B	128	SER
1	B	147	HIS
1	B	152	THR
1	B	164	ARG
1	B	166	VAL
1	B	175	ILE
2	C	96	LYS
2	C	101	HIS
2	C	108	VAL
2	C	110	GLN
2	C	111	THR
2	C	113	ILE
2	C	116	LYS
2	C	119	LEU
2	C	146	LYS
2	C	163	GLU
2	C	166	LYS
2	C	171	SER
2	C	172	THR
2	C	175	SER
2	C	206	ASN
2	C	207	ILE
2	C	211	GLN
2	C	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	B	156	GLN
2	C	102	GLN
2	C	174	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 ⓘ

4 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	D	1	1,3	14,14,15	0.50	0	17,19,21	1.22	1 (5%)
3	NAG	D	2	3	14,14,15	0.78	0	17,19,21	1.94	4 (23%)
3	NAG	E	1	3,2	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
3	NAG	E	2	3	14,14,15	0.61	0	17,19,21	1.67	4 (23%)

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	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	4.52	118.25	112.19
3	D	2	NAG	C3-C4-C5	-3.53	103.83	110.23
3	E	1	NAG	C4-C3-C2	-3.27	106.22	111.02
3	E	1	NAG	O5-C1-C2	-3.11	106.47	111.29
3	D	2	NAG	O4-C4-C5	2.97	116.63	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C4-C3-C2	2.79	115.11	111.02
3	E	2	NAG	O5-C5-C4	-2.78	104.05	110.83
3	E	2	NAG	O3-C3-C2	-2.42	104.38	109.40
3	D	1	NAG	O5-C5-C6	-2.41	102.97	107.66
3	E	2	NAG	C1-C2-N2	-2.29	106.82	110.43
3	D	2	NAG	C4-C3-C2	-2.07	107.98	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

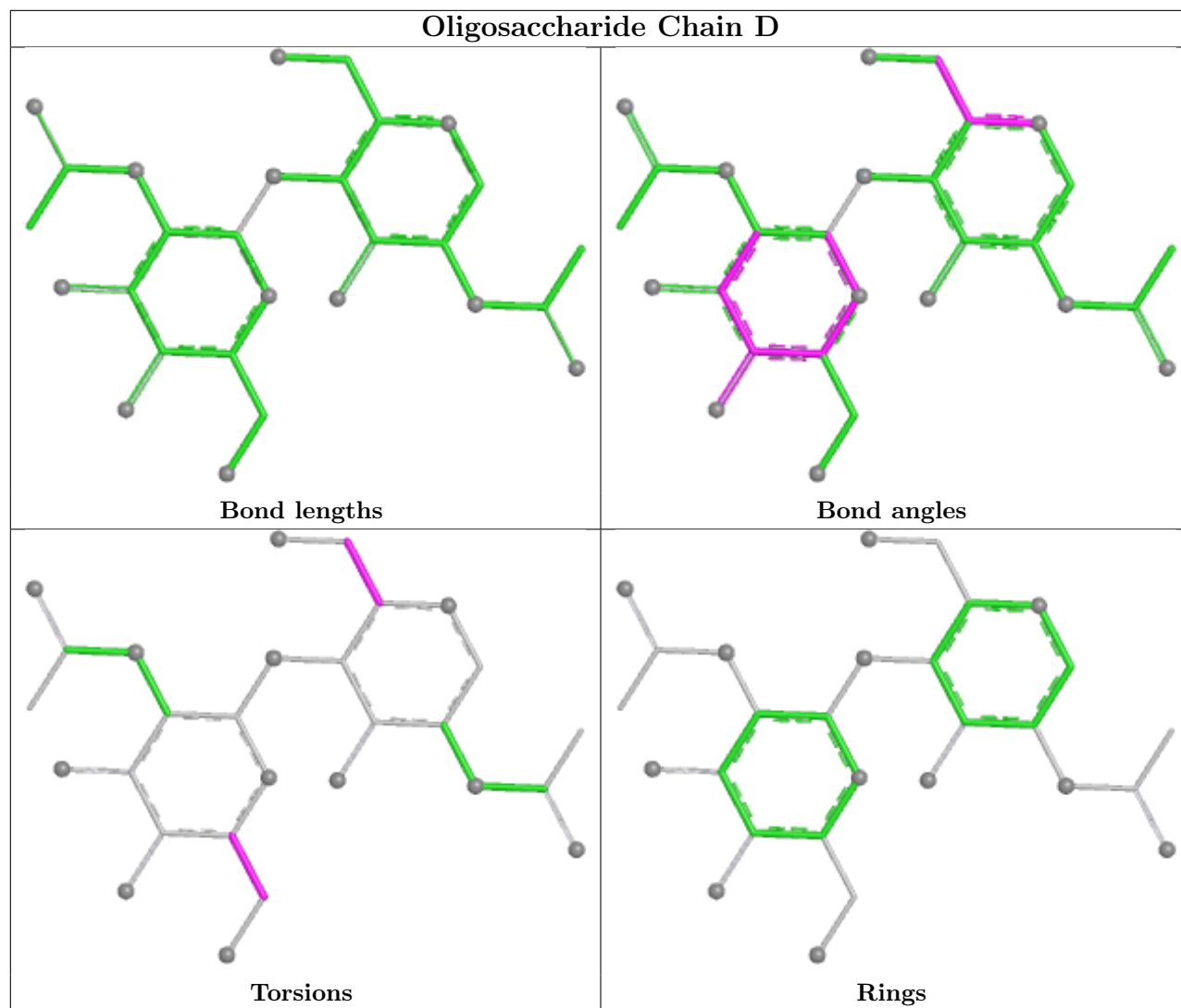
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

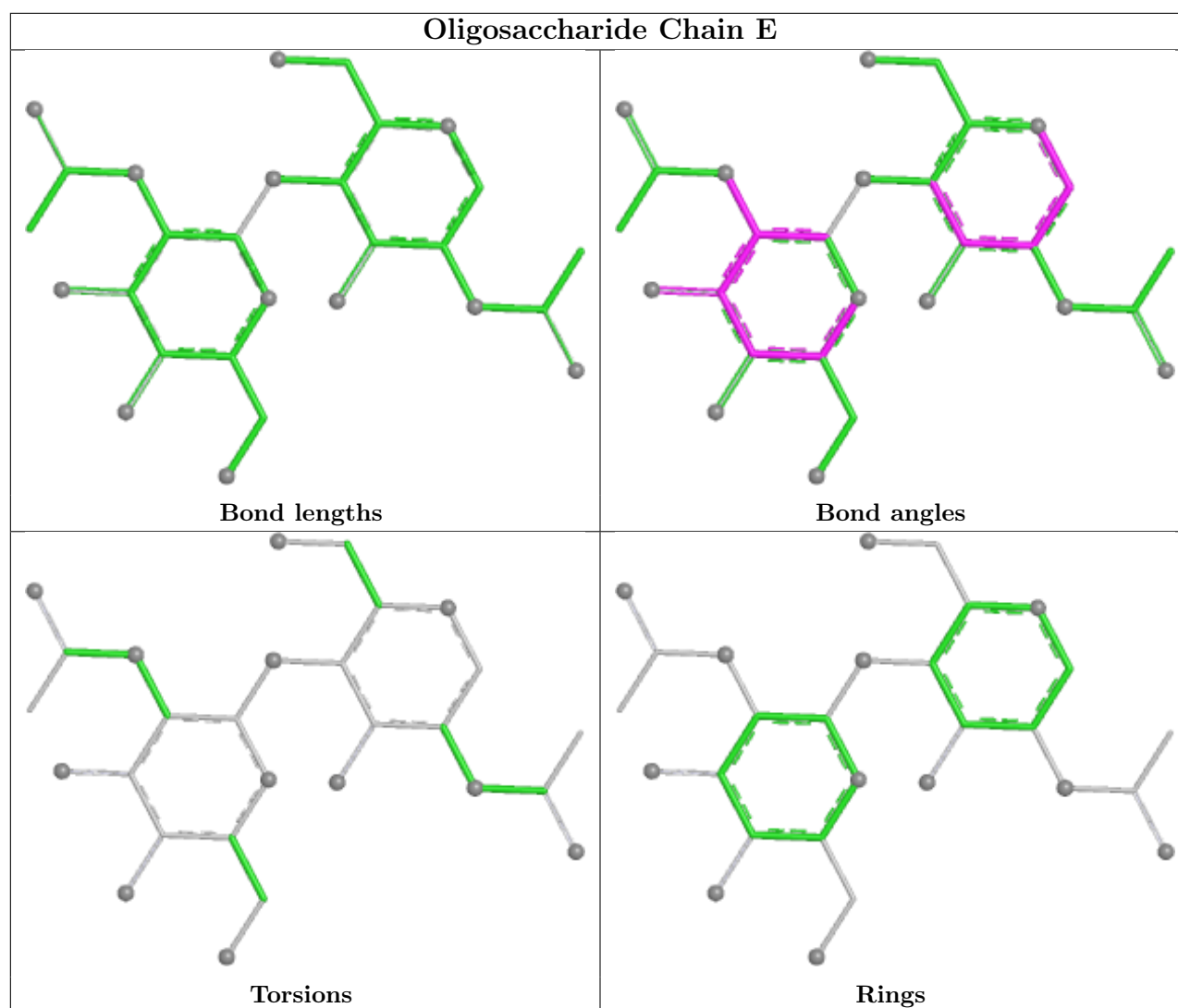
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	NAG	A	301	1	14,14,15	0.75	0	17,19,21	1.30	3 (17%)
4	NAG	C	301	2	14,14,15	0.96	2 (14%)	17,19,21	1.91	6 (35%)
4	NAG	B	301	1	14,14,15	1.35	2 (14%)	17,19,21	2.79	8 (47%)

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	A	301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	301	2	-	0/6/23/26	0/1/1/1
4	NAG	B	301	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	NAG	C3-C2	2.86	1.58	1.52
4	B	301	NAG	O4-C4	2.31	1.48	1.43
4	C	301	NAG	C3-C2	2.10	1.56	1.52
4	C	301	NAG	C1-C2	2.03	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAG	C1-O5-C5	5.65	119.76	112.19
4	B	301	NAG	O3-C3-C2	4.69	119.15	109.40
4	B	301	NAG	O5-C1-C2	-4.28	104.66	111.29
4	C	301	NAG	C1-O5-C5	4.27	117.91	112.19
4	B	301	NAG	C1-C2-N2	-4.20	103.81	110.43
4	A	301	NAG	C1-O5-C5	3.88	117.39	112.19
4	B	301	NAG	C3-C4-C5	-3.36	104.14	110.23
4	B	301	NAG	O4-C4-C5	3.14	117.06	109.32
4	C	301	NAG	C1-C2-N2	-3.09	105.56	110.43
4	B	301	NAG	O3-C3-C4	-2.57	104.33	110.38
4	A	301	NAG	C3-C4-C5	2.49	114.75	110.23
4	B	301	NAG	C2-N2-C7	2.47	126.22	122.90
4	C	301	NAG	C6-C5-C4	-2.43	107.06	113.02
4	C	301	NAG	C4-C3-C2	2.38	114.50	111.02
4	C	301	NAG	C3-C4-C5	-2.15	106.33	110.23
4	A	301	NAG	C2-N2-C7	2.09	125.71	122.90
4	C	301	NAG	O4-C4-C3	2.08	115.29	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	NAG	O5-C5-C6-O6
4	B	301	NAG	O5-C5-C6-O6
4	B	301	NAG	C4-C5-C6-O6
4	A	301	NAG	C4-C5-C6-O6

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	129/133 (96%)	-0.23	2 (1%) 70 47	84, 105, 146, 190	0
1	B	122/133 (91%)	-0.26	0 100 100	86, 113, 148, 185	0
2	C	121/151 (80%)	-0.32	0 100 100	86, 112, 144, 166	0
All	All	372/417 (89%)	-0.27	2 (0%) 87 72	84, 111, 148, 190	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	THR	2.8
1	A	74	ILE	2.6

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.

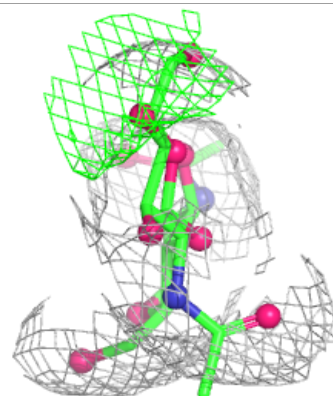
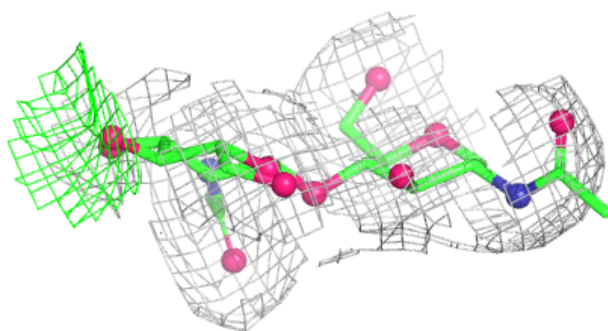
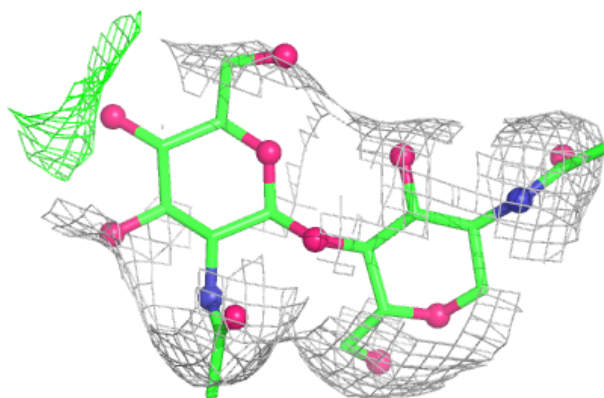
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.77	0.13	126,176,212,227	0
3	NAG	D	2	14/15	0.82	0.10	111,154,169,185	0
3	NAG	E	1	14/15	0.91	0.07	117,135,147,149	0
3	NAG	D	1	14/15	0.95	0.08	101,119,124,135	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

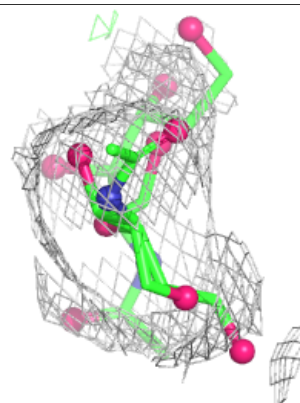
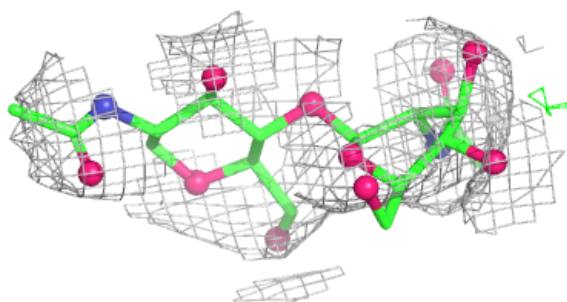
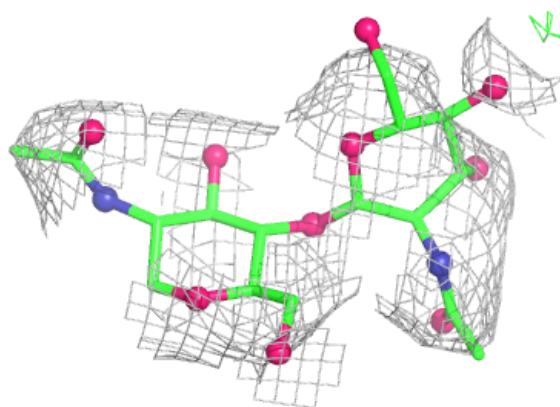
Electron density around Chain D:

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



Electron density around Chain E:

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



6.4 Ligands [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
4	NAG	A	301	14/15	0.33	0.09	160,213,223,234	0
4	NAG	C	301	14/15	0.81	0.10	143,153,169,172	0
4	NAG	B	301	14/15	0.86	0.10	106,121,129,132	0
5	ZN	A	302	1/1	1.00	0.01	106,106,106,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.