



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:46 PM UTC

PDB ID : 3VKF / pdb_00003vkf
Title : Crystal Structure of Neurexin 1beta/Neurologin 1 complex
Authors : Tanaka, H.; Miyazaki, N.; Nogi, T.; Iwasaki, K.; Takagi, J.
Deposited on : 2011-11-15
Resolution : 3.30 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

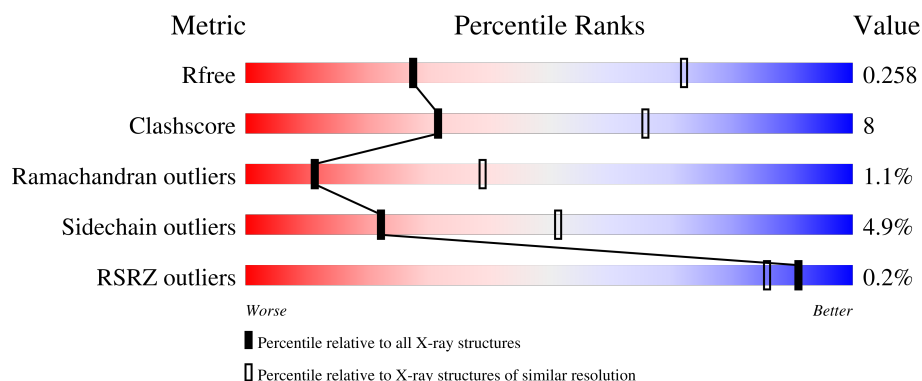
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	585	73% 21% ..
1	B	585	74% 15% • 10%
2	C	181	70% 25% ..
2	D	181	% 71% 26% ..
3	E	3	33% 67%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11320 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 Neuroligin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4399	2820	739	822	18			
1	B	527	Total	C	N	O	S	0	0	0
			4144	2666	688	774	16			

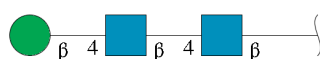
- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1354	853	241	259	1			
2	D	177	Total	C	N	O	S	0	0	0
			1354	853	241	259	1			

There are 6 discrepancies between the modelled and reference sequences:

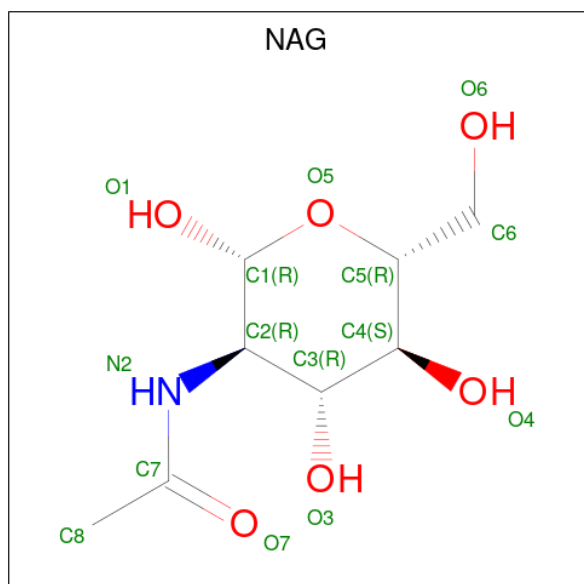
Chain	Residue	Modelled	Actual	Comment	Reference
C	81	GLY	-	expression tag	UNP Q28142
C	82	SER	-	expression tag	UNP Q28142
C	291	SER	-	expression tag	UNP Q28142
D	81	GLY	-	expression tag	UNP Q28142
D	82	SER	-	expression tag	UNP Q28142
D	291	SER	-	expression tag	UNP Q28142

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

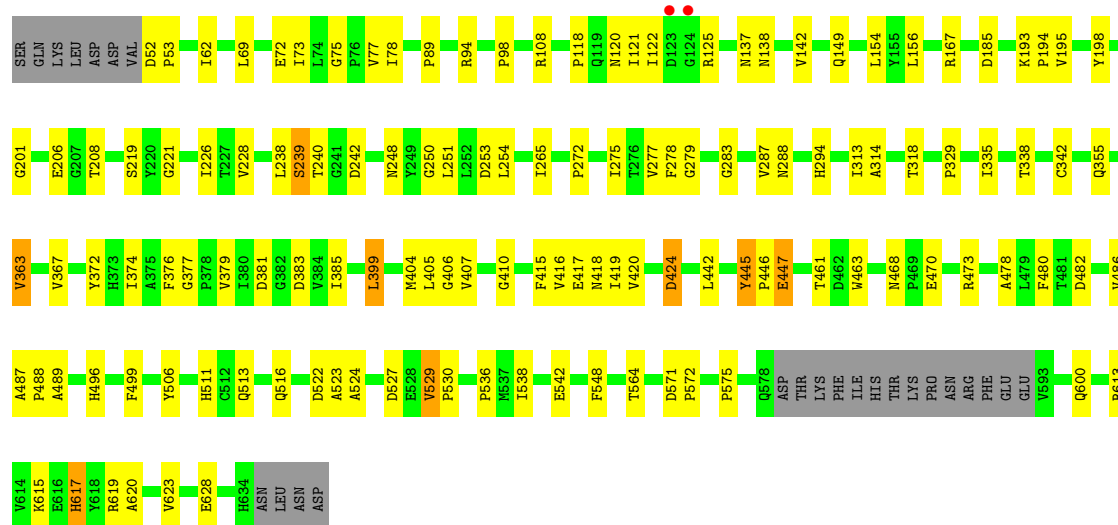
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

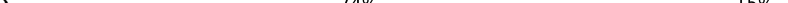
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

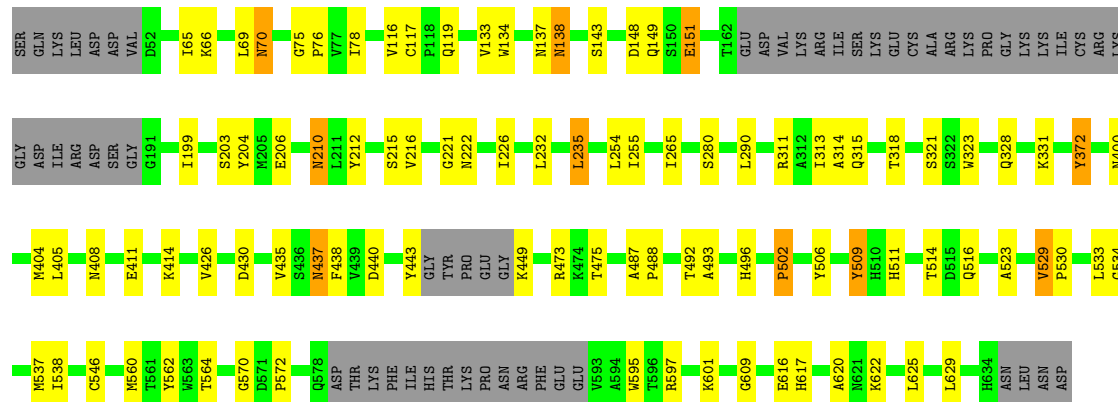
- Molecule 1: Neuroligin-1

Chain A: 73% 21% ..



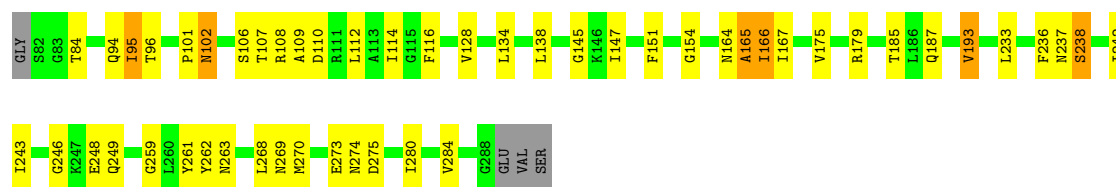
- Molecule 1: Neuroligin-1

Chain B:  74% 15% 10%



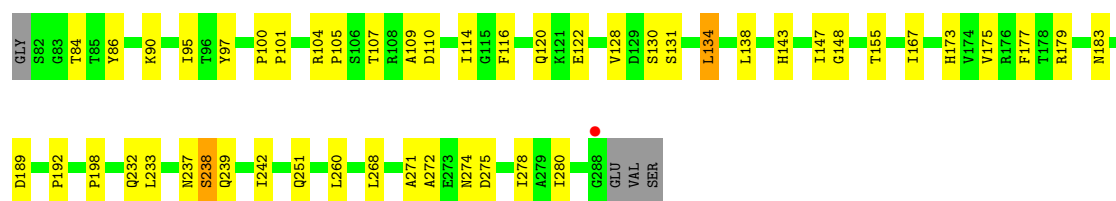
- Molecule 2: Neurexin-1-beta

Chain C:  70% 25% ..

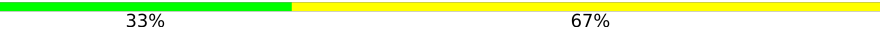


• Molecule 2: Neurexin-1-beta

Chain D:  71% 26% ..



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

Chain E:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.26Å 95.19Å 120.40Å 90.00° 108.62° 90.00°	Depositor
Resolution (Å)	48.91 – 3.30 48.91 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.91-3.30) 96.7 (48.91-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.287 (Not available) , 0.258	Depositor DCC
R_{free} test set	2586 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11320	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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, BMA, CA

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	0.50	1/4521 (0.0%)	0.83	6/6165 (0.1%)
1	B	0.49	1/4261 (0.0%)	0.83	2/5819 (0.0%)
2	C	0.51	0/1379	0.81	1/1868 (0.1%)
2	D	0.48	0/1379	0.82	1/1868 (0.1%)
All	All	0.50	2/11540 (0.0%)	0.83	10/15720 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	VAL	CA-CB	6.15	1.57	1.54
1	B	529	VAL	CA-CB	5.85	1.57	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ILE	CA-C-N	6.50	125.73	118.97
1	A	385	ILE	C-N-CA	6.50	125.73	118.97
1	B	75	GLY	CA-C-N	6.01	127.36	119.84
1	B	75	GLY	C-N-CA	6.01	127.36	119.84
1	A	75	GLY	CA-C-N	5.81	126.14	119.92
1	A	75	GLY	C-N-CA	5.81	126.14	119.92
1	A	571	ASP	CA-C-N	5.58	125.25	119.56
1	A	571	ASP	C-N-CA	5.58	125.25	119.56
2	C	107	THR	N-CA-C	5.52	116.90	108.52
2	D	274	ASN	N-CA-C	5.20	118.51	111.17

There are no chirality outliers.

There are no planarity outliers.

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	4399	0	4269	69	0
1	B	4144	0	4005	47	0
2	C	1354	0	1343	39	0
2	D	1354	0	1343	29	0
3	E	39	0	34	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	11320	0	11020	180	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 (180) 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:A:445:TYR:HB2	1:A:446:PRO:HD3	1.32	1.07
1:A:445:TYR:CB	1:A:446:PRO:HD3	2.01	0.89
1:A:445:TYR:HB2	1:A:446:PRO:CD	2.02	0.89
2:D:147:ILE:H	2:D:167:ILE:HD13	1.40	0.86
1:A:314:ALA:HB3	1:A:405:LEU:HD23	1.63	0.81
1:B:514:THR:HB	1:B:546:CYS:HB3	1.66	0.76
2:C:114:ILE:HG22	2:C:175:VAL:HG12	1.69	0.74
2:D:138:LEU:HD11	2:D:177:PHE:CE2	2.24	0.73
1:A:329:PRO:HB3	1:A:379:VAL:HG11	1.68	0.73
1:A:201:GLY:HA3	1:A:283:GLY:N	2.04	0.73
2:C:269:ASN:O	2:C:273:GLU:HG2	1.89	0.71
1:A:201:GLY:HA3	1:A:283:GLY:H	1.56	0.69
1:A:288:ASN:HD22	1:A:318:THR:HA	1.57	0.69
2:C:95:ILE:HG22	2:C:280:ILE:HG23	1.76	0.67
1:B:134:TRP:O	1:B:138:ASN:HB2	1.96	0.66
1:A:446:PRO:O	1:A:447:GLU:HB2	1.96	0.66
1:A:478:ALA:HB1	1:A:619:ARG:HH22	1.60	0.65
1:B:408:ASN:O	1:B:411:GLU:HG2	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:ALA:HA	2:D:179:ARG:O	1.98	0.64
2:D:110:ASP:CG	2:D:179:ARG:HH21	2.06	0.64
2:C:138:LEU:HD12	2:C:151:PHE:HB3	1.81	0.63
2:D:183:ASN:HD22	2:D:198:PRO:HD2	1.64	0.63
1:B:69:LEU:HD21	1:B:215:SER:HB3	1.81	0.62
1:A:381:ASP:OD2	1:A:383:ASP:HB3	2.00	0.62
1:A:511:HIS:HB3	1:A:523:ALA:HA	1.80	0.61
1:A:288:ASN:ND2	1:A:318:THR:HA	2.16	0.60
1:B:313:ILE:HG12	1:B:404:MET:HB3	1.83	0.60
1:A:277:VAL:HG12	1:A:287:VAL:HG22	1.81	0.60
1:A:511:HIS:HE1	1:A:513:GLN:HE21	1.49	0.60
1:B:321:SER:HG	1:B:323:TRP:CD1	2.20	0.60
2:C:116:PHE:HZ	2:C:167:ILE:HG21	1.67	0.58
1:B:616:GLU:HG2	1:B:617:HIS:CD2	2.38	0.58
2:C:187:GLN:HB2	2:C:193:VAL:HG13	1.86	0.58
2:C:246:GLY:HA2	2:C:249:GLN:OE1	2.03	0.57
2:C:270:MET:O	2:C:275:ASP:HB2	2.04	0.57
1:A:118:PRO:HB2	1:A:363:VAL:HG21	1.87	0.56
2:C:101:PRO:HB2	2:C:102:ASN:HD22	1.70	0.56
2:D:122:GLU:HG2	2:D:143:HIS:HA	1.87	0.56
1:A:617:HIS:HB3	1:A:620:ALA:HB2	1.86	0.56
2:D:110:ASP:HB2	2:D:179:ARG:HB3	1.88	0.56
2:D:275:ASP:HB3	2:D:278:ILE:HD12	1.87	0.56
1:A:407:VAL:HG21	1:A:486:VAL:HG22	1.87	0.55
2:C:96:THR:HG23	2:C:243:ILE:HD13	1.87	0.55
2:D:107:THR:HG22	2:D:239:GLN:HE22	1.72	0.54
1:B:226:ILE:HD11	1:B:265:ILE:HD13	1.89	0.54
2:D:97:TYR:HD1	2:D:278:ILE:HG13	1.73	0.54
2:C:95:ILE:HD11	2:C:268:LEU:HD23	1.89	0.54
1:B:221:GLY:HA3	1:B:564:THR:HG21	1.90	0.53
1:B:443:TYR:C	1:B:449:LYS:HE3	2.33	0.53
1:B:328:GLN:NE2	1:B:331:LYS:HD2	2.24	0.53
1:A:226:ILE:HD11	1:A:265:ILE:HD13	1.90	0.53
1:A:399:LEU:HD11	2:C:108:ARG:HH22	1.74	0.52
2:C:138:LEU:HB2	2:C:236:PHE:HE2	1.75	0.52
1:A:251:LEU:HA	1:A:254:LEU:HD12	1.91	0.52
1:B:70:ASN:HD22	1:B:538:ILE:HG21	1.74	0.52
2:C:106:SER:HA	2:C:236:PHE:O	2.09	0.52
1:A:248:ASN:OD1	1:A:251:LEU:HD12	2.10	0.51
1:A:77:VAL:HG22	1:A:219:SER:HB3	1.92	0.51
2:D:84:THR:HG21	2:D:272:ALA:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ALA:HA	1:A:623:VAL:HG13	1.93	0.51
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.91	0.51
1:A:318:THR:HG21	1:A:489:ALA:HA	1.92	0.50
1:A:374:ILE:HD12	1:A:377:GLY:HA3	1.93	0.50
1:B:216:VAL:HG11	1:B:534:GLY:O	2.11	0.50
2:C:95:ILE:HB	2:C:280:ILE:HG12	1.92	0.50
1:B:625:LEU:HD12	1:B:629:LEU:HD23	1.92	0.50
1:A:415:PHE:CD2	1:A:480:PHE:HB2	2.47	0.50
2:C:102:ASN:HD22	2:C:102:ASN:N	2.09	0.50
2:D:116:PHE:HZ	2:D:167:ILE:CG2	2.25	0.50
2:D:107:THR:HG21	2:D:110:ASP:OD1	2.12	0.50
2:C:179:ARG:NH2	2:C:236:PHE:HB2	2.27	0.50
1:A:404:MET:HE2	1:A:572:PRO:HG3	1.94	0.49
1:B:280:SER:HA	1:B:315:GLN:O	2.12	0.49
2:C:147:ILE:H	2:C:167:ILE:HD13	1.78	0.49
1:B:509:TYR:CE1	1:B:609:GLY:HA3	2.48	0.49
1:A:52:ASP:N	1:A:53:PRO:HD3	2.26	0.49
1:B:617:HIS:HB3	1:B:620:ALA:HB2	1.94	0.49
1:A:120:ASN:HD21	1:A:125:ARG:HH22	1.60	0.48
1:A:613:ARG:HD2	1:A:615:LYS:HG2	1.94	0.48
2:C:112:LEU:HA	2:C:261:TYR:O	2.13	0.48
1:A:470:GLU:O	1:A:473:ARG:HB3	2.14	0.48
1:B:314:ALA:HB3	1:B:405:LEU:HD23	1.96	0.48
1:B:137:ASN:HD22	1:B:516:GLN:HG2	1.78	0.47
2:D:237:ASN:O	2:D:238:SER:C	2.57	0.47
1:A:294:HIS:HD2	2:C:108:ARG:CD	2.27	0.47
1:B:435:VAL:O	1:B:438:PHE:HB3	2.14	0.47
1:A:221:GLY:HA3	1:A:564:THR:HG21	1.97	0.47
1:A:542:GLU:H	1:A:542:GLU:CD	2.22	0.47
2:C:94:GLN:HE22	2:C:248:GLU:HB2	1.80	0.47
2:D:155:THR:HG23	2:D:233:LEU:HG	1.95	0.47
1:A:238:LEU:HD12	1:A:376:PHE:HE1	1.79	0.47
2:D:128:VAL:HG22	2:D:242:ILE:HG12	1.96	0.47
2:D:198:PRO:HB2	2:D:232:GLN:HE22	1.78	0.47
1:A:53:PRO:HB3	1:A:78:ILE:HD13	1.97	0.47
1:B:116:VAL:HG23	1:B:149:GLN:HG2	1.96	0.47
1:B:212:TYR:HD1	1:B:533:LEU:HD11	1.79	0.46
2:C:114:ILE:HG22	2:C:175:VAL:CG1	2.43	0.46
1:A:137:ASN:HB3	1:A:516:GLN:NE2	2.30	0.46
2:D:173:HIS:ND1	2:D:189:ASP:OD1	2.37	0.46
1:A:250:GLY:O	1:A:253:ASP:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:TYR:CE1	1:A:279:GLY:HA2	2.50	0.46
1:A:313:ILE:HG12	1:A:404:MET:HB3	1.98	0.46
1:B:66:LYS:HE2	1:B:76:PRO:HB3	1.97	0.46
1:A:120:ASN:ND2	1:A:125:ARG:HH22	2.14	0.46
1:A:98:PRO:HG3	1:A:253:ASP:HA	1.98	0.46
1:A:239:SER:HB3	1:A:329:PRO:HB2	1.98	0.46
1:B:506:TYR:HB3	1:B:595:TRP:CZ2	2.52	0.45
2:C:154:GLY:HA3	2:C:233:LEU:HD12	1.99	0.45
1:B:616:GLU:HG2	1:B:617:HIS:HD2	1.80	0.45
1:B:437:ASN:HA	1:B:440:ASP:HB2	1.98	0.45
1:A:482:ASP:OD1	1:A:619:ARG:NH2	2.49	0.45
1:B:426:VAL:HG23	1:B:473:ARG:HG3	1.99	0.45
2:C:147:ILE:N	2:C:167:ILE:HD13	2.31	0.45
1:A:156:LEU:HD22	1:A:228:VAL:HG22	1.97	0.45
1:A:198:TYR:HB2	1:A:278:PHE:CZ	2.52	0.45
1:A:314:ALA:HB3	1:A:405:LEU:CD2	2.40	0.44
1:B:487:ALA:HB3	1:B:488:PRO:HD3	1.98	0.44
2:C:164:ASN:O	2:C:165:ALA:HB2	2.16	0.44
1:A:529:VAL:N	1:A:530:PRO:HD2	2.31	0.44
1:B:405:LEU:HD12	1:B:493:ALA:HB2	1.99	0.44
2:C:145:GLY:HA3	2:C:166:ILE:HG12	2.00	0.44
1:B:199:ILE:HG12	1:B:254:LEU:HD22	1.97	0.44
1:A:198:TYR:HA	1:A:278:PHE:O	2.17	0.44
1:A:536:PRO:HG3	1:A:548:PHE:CD2	2.52	0.44
1:B:372:TYR:CD1	1:B:372:TYR:N	2.84	0.44
1:B:562:TYR:HD1	1:B:572:PRO:HB2	1.82	0.44
2:C:116:PHE:CZ	2:C:167:ILE:HG21	2.52	0.44
2:C:237:ASN:O	2:C:238:SER:C	2.60	0.44
1:A:406:GLY:HA3	1:A:506:TYR:CE2	2.52	0.43
2:C:179:ARG:HH22	2:C:236:PHE:HB2	1.82	0.43
1:B:414:LYS:HE2	1:B:414:LYS:HA	2.00	0.43
1:A:138:ASN:O	1:A:142:VAL:HG23	2.19	0.43
1:A:420:VAL:HG12	1:A:424:ASP:HA	2.00	0.43
2:C:94:GLN:HE21	2:C:248:GLU:H	1.67	0.43
1:B:511:HIS:HB3	1:B:523:ALA:HA	2.00	0.43
1:A:446:PRO:O	1:A:447:GLU:CB	2.65	0.43
1:B:117:CYS:O	1:B:119:GLN:HG2	2.19	0.43
1:B:203:SER:O	1:B:204:TYR:HB2	2.19	0.43
2:D:95:ILE:HG12	2:D:280:ILE:HG12	2.00	0.43
1:A:89:PRO:HG3	1:A:154:LEU:HD11	2.01	0.42
1:B:492:THR:HG22	1:B:496:HIS:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:PHE:CZ	2:D:167:ILE:HG22	2.53	0.42
1:B:66:LYS:HG3	1:B:78:ILE:HD13	2.01	0.42
1:B:622:LYS:O	1:B:625:LEU:HB3	2.18	0.42
2:C:109:ALA:HA	2:C:179:ARG:O	2.19	0.42
2:D:134:LEU:HD12	2:D:134:LEU:N	2.34	0.42
2:D:130:SER:HA	2:D:239:GLN:HA	2.00	0.42
2:D:86:TYR:HD2	2:D:268:LEU:HD22	1.84	0.42
1:A:410:GLY:O	1:A:524:ALA:HA	2.20	0.42
2:D:114:ILE:HD12	2:D:260:LEU:HD13	2.02	0.42
2:C:128:VAL:HG22	2:C:242:ILE:HG12	2.02	0.42
2:D:104:ARG:HA	2:D:105:PRO:HD3	1.82	0.42
1:A:445:TYR:CB	1:A:446:PRO:CD	2.71	0.42
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.97	0.42
1:A:399:LEU:HD11	2:C:108:ARG:NH2	2.34	0.42
1:A:94:ARG:HD2	1:A:355:GLN:HA	2.02	0.41
1:B:255:ILE:HD11	1:B:290:LEU:HD22	2.01	0.41
1:B:311:ARG:HD3	1:B:570:GLY:HA2	2.02	0.41
1:A:272:PRO:HA	1:A:275:ILE:HD11	2.02	0.41
2:C:110:ASP:OD2	2:C:179:ARG:NE	2.48	0.41
1:A:62:ILE:HG22	1:A:108:ARG:HG2	2.02	0.41
2:C:128:VAL:HB	2:C:138:LEU:HB3	2.03	0.41
1:A:482:ASP:HA	1:A:486:VAL:HB	2.03	0.41
2:C:116:PHE:HZ	2:C:167:ILE:CG2	2.34	0.41
2:D:116:PHE:HZ	2:D:167:ILE:HG21	1.84	0.41
1:A:416:VAL:O	1:A:418:ASN:N	2.39	0.41
2:D:100:PRO:HA	2:D:101:PRO:HD3	1.94	0.41
1:A:468:ASN:HD21	1:A:470:GLU:HB2	1.86	0.41
1:B:210:ASN:OD1	1:B:210:ASN:N	2.54	0.41
1:B:502:PRO:HA	1:B:597:ARG:HD2	2.02	0.41
1:B:537:MET:HE3	1:B:560:MET:CE	2.50	0.41
2:D:147:ILE:HG13	2:D:148:GLY:N	2.36	0.41
1:A:499:PHE:CD2	2:C:134:LEU:HD21	2.57	0.40
1:A:461:THR:O	1:A:463:TRP:CD1	2.74	0.40
1:B:151:GLU:HG2	1:B:235:LEU:HD21	2.02	0.40
1:B:529:VAL:N	1:B:530:PRO:HD2	2.37	0.40
2:C:110:ASP:OD2	2:C:179:ARG:NH2	2.53	0.40
2:C:262:TYR:O	2:C:263:ASN:C	2.64	0.40
1:B:70:ASN:HD22	1:B:538:ILE:CG2	2.34	0.40
2:D:271:ALA:HB2	2:D:278:ILE:HG21	2.04	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	556/585 (95%)	500 (90%)	47 (8%)	9 (2%)	7	31
1	B	519/585 (89%)	480 (92%)	38 (7%)	1 (0%)	43	71
2	C	175/181 (97%)	156 (89%)	16 (9%)	3 (2%)	7	30
2	D	175/181 (97%)	158 (90%)	15 (9%)	2 (1%)	11	39
All	All	1425/1532 (93%)	1294 (91%)	116 (8%)	15 (1%)	11	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	TYR
1	A	447	GLU
2	C	165	ALA
2	D	238	SER
1	A	73	ILE
1	A	242	ASP
2	C	238	SER
1	A	417	GLU
1	A	527	ASP
1	A	72	GLU
1	A	617	HIS
2	C	259	GLY
1	B	502	PRO
2	D	192	PRO
1	A	575	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	478/503 (95%)	452 (95%)	26 (5%)	20	49
1	B	451/503 (90%)	431 (96%)	20 (4%)	25	54
2	C	143/146 (98%)	135 (94%)	8 (6%)	19	47
2	D	143/146 (98%)	137 (96%)	6 (4%)	26	55
All	All	1215/1298 (94%)	1155 (95%)	60 (5%)	22	51

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	121	ILE
1	A	122	ILE
1	A	149	GLN
1	A	167	ARG
1	A	185	ASP
1	A	195	VAL
1	A	206	GLU
1	A	208	THR
1	A	239	SER
1	A	240	THR
1	A	335	ILE
1	A	338	THR
1	A	342	CYS
1	A	363	VAL
1	A	367	VAL
1	A	372	TYR
1	A	399	LEU
1	A	419	ILE
1	A	424	ASP
1	A	442	LEU
1	A	496	HIS
1	A	522	ASP
1	A	538	ILE
1	A	600	GLN
1	A	628	GLU
1	B	65	ILE
1	B	70	ASN
1	B	133	VAL
1	B	138	ASN
1	B	143	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	148	ASP
1	B	151	GLU
1	B	206	GLU
1	B	210	ASN
1	B	222	ASN
1	B	232	LEU
1	B	235	LEU
1	B	318	THR
1	B	372	TYR
1	B	400	ASN
1	B	430	ASP
1	B	437	ASN
1	B	475	THR
1	B	509	TYR
1	B	601	LYS
2	C	84	THR
2	C	95	ILE
2	C	102	ASN
2	C	166	ILE
2	C	185	THR
2	C	193	VAL
2	C	274	ASN
2	C	284	VAL
2	D	90	LYS
2	D	120	GLN
2	D	131	SER
2	D	134	LEU
2	D	175	VAL
2	D	251	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	79	GLN
1	A	120	ASN
1	A	229	ASN
1	A	288	ASN
1	A	294	HIS
1	A	409	GLN
1	A	467	HIS
1	A	468	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	496	HIS
1	A	511	HIS
1	A	513	GLN
1	A	516	GLN
1	A	600	GLN
1	A	603	GLN
1	B	70	ASN
1	B	137	ASN
1	B	229	ASN
1	B	243	GLN
1	B	288	ASN
1	B	328	GLN
1	B	409	GLN
1	B	437	ASN
1	B	496	HIS
1	B	511	HIS
1	B	513	GLN
1	B	600	GLN
2	C	94	GLN
2	C	102	ASN
2	C	144	GLN
2	C	164	ASN
2	C	183	ASN
2	D	94	GLN
2	D	102	ASN
2	D	144	GLN
2	D	183	ASN
2	D	232	GLN
2	D	239	GLN
2	D	249	GLN
2	D	254	GLN
2	D	269	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

3 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	E	1	1,3	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
3	NAG	E	2	3	14,14,15	0.48	0	17,19,21	0.85	0
3	BMA	E	3	3	11,11,12	0.55	0	15,15,17	1.11	2 (13%)

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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	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	E	3	BMA	C1-C2-C3	3.02	114.05	109.64
3	E	1	NAG	C4-C3-C2	2.89	115.25	111.02
3	E	3	BMA	C2-C3-C4	2.11	114.57	110.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2

Continued on next page...

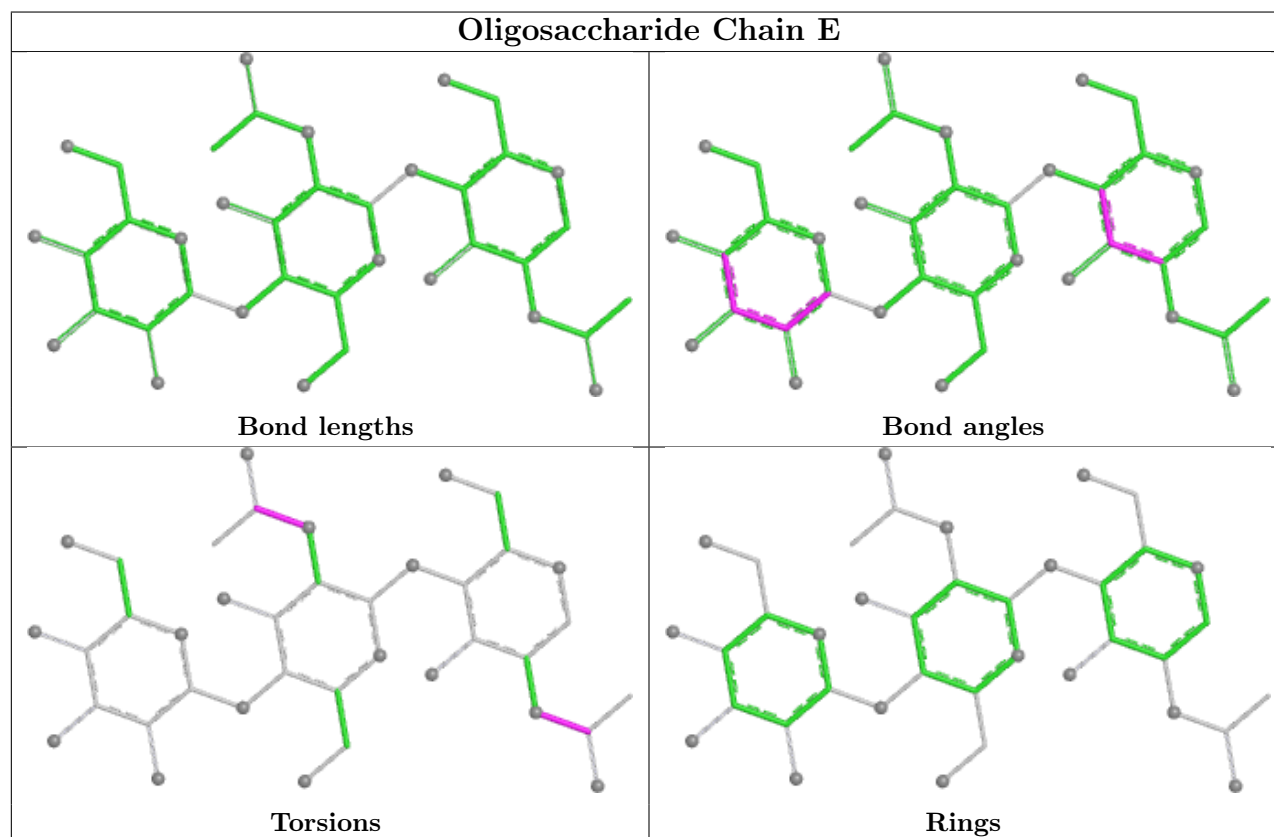
Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O7-C7-N2-C2

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	2001	1	14,14,15	0.48	0	17,19,21	0.70	0
4	NAG	B	2001	1	14,14,15	0.58	0	17,19,21	0.97	1 (5%)

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	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	NAG	C4-C3-C2	2.91	115.29	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2001	NAG	C8-C7-N2-C2
4	B	2001	NAG	O7-C7-N2-C2
4	A	2001	NAG	C8-C7-N2-C2
4	A	2001	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	560/585 (95%)	-0.12	2 (0%) 88 79	36, 59, 87, 119	0
1	B	527/585 (90%)	-0.07	0 100 100	48, 72, 96, 117	0
2	C	177/181 (97%)	-0.22	0 100 100	43, 60, 76, 87	0
2	D	177/181 (97%)	-0.06	1 (0%) 85 73	54, 75, 101, 121	0
All	All	1441/1532 (94%)	-0.11	3 (0%) 91 86	36, 66, 94, 121	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ASP	2.7
1	A	124	GLY	2.2
2	D	288	GLY	2.1

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

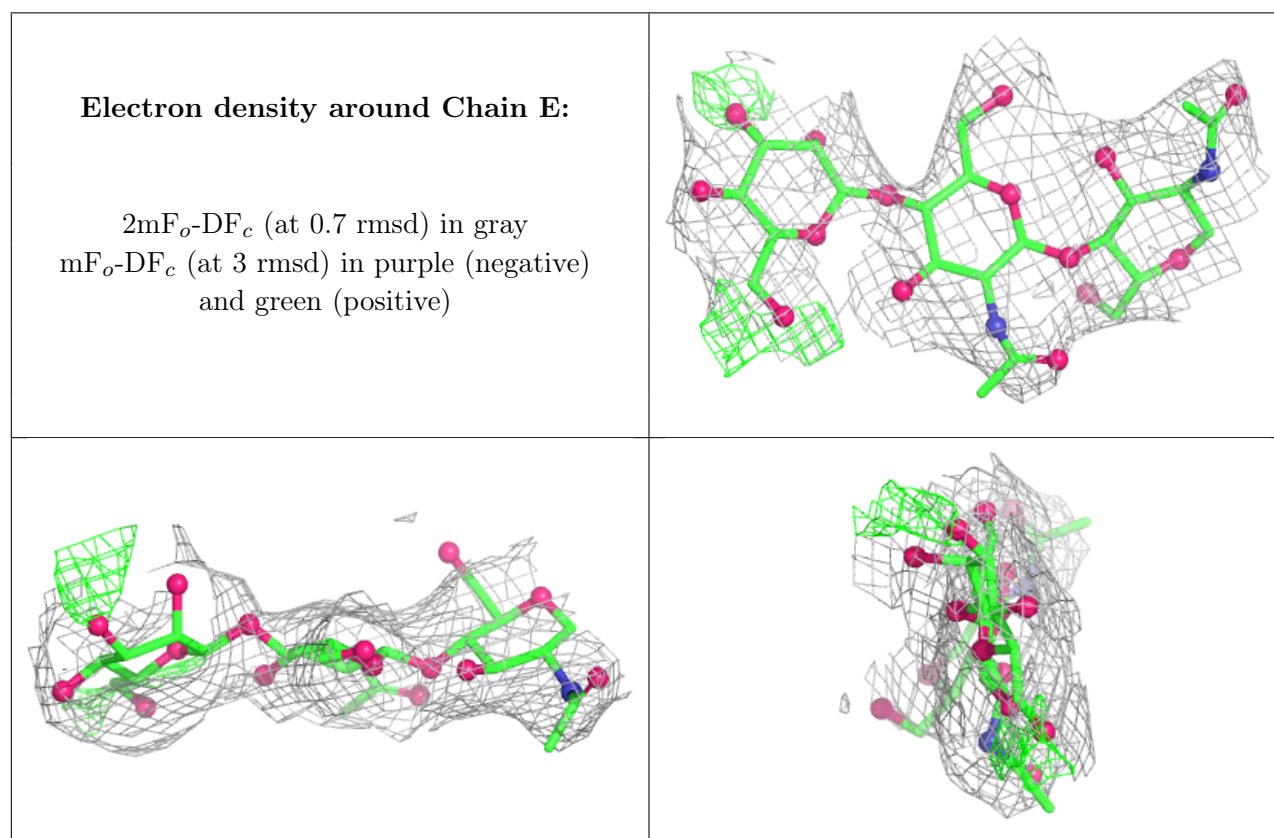
There are no non-standard protein/DNA/RNA residues in this entry.

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	BMA	E	3	11/12	0.64	0.15	111,114,119,122	0
3	NAG	E	2	14/15	0.76	0.10	98,103,109,109	0
3	NAG	E	1	14/15	0.81	0.09	89,94,97,98	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 ⓘ

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	NAG	B	2001	14/15	0.78	0.09	98,108,114,119	0
4	NAG	A	2001	14/15	0.86	0.09	77,83,88,90	0
5	CA	C	2001	1/1	0.95	0.07	68,68,68,68	0
5	CA	D	2001	1/1	0.96	0.06	70,70,70,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.