Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 03:35 pm GMT

PDB ID	:	30PU / pdb_000030pu
Title	:	Structure of a TrkB:BDNF complex
Authors	:	Briggs, D.C.; McDonald, N.Q.
Deposited on	:	2026-05-07
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

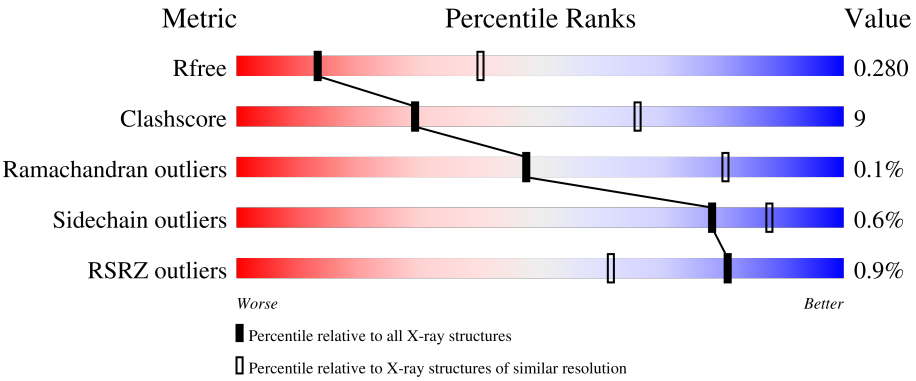
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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 <=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	392	73% 17% 10%
1	C	392	73% 17% 10%
2	B	119	81% 17%
2	D	119	82% 15%
3	E	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14646 atoms, of which 7237 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 BDNF/NT-3 growth factors receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	353	Total	C	H	N	O	S	0	0	0
			5408	1727	2661	470	532	18			
1	C	351	Total	C	H	N	O	S	0	0	0
			5386	1719	2654	468	527	18			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q16620
A	2	ALA	-	expression tag	UNP Q16620
A	95	GLN	ASN	engineered mutation	UNP Q16620
A	121	GLN	ASN	engineered mutation	UNP Q16620
A	178	GLN	ASN	engineered mutation	UNP Q16620
A	241	GLN	ASN	conflict	UNP Q16620
A	280	GLN	ASN	engineered mutation	UNP Q16620
A	325	SER	ASN	engineered mutation	UNP Q16620
A	384	ALA	-	expression tag	UNP Q16620
A	385	ALA	-	expression tag	UNP Q16620
A	386	ALA	-	expression tag	UNP Q16620
A	387	HIS	-	expression tag	UNP Q16620
A	388	HIS	-	expression tag	UNP Q16620
A	389	HIS	-	expression tag	UNP Q16620
A	390	HIS	-	expression tag	UNP Q16620
A	391	HIS	-	expression tag	UNP Q16620
A	392	HIS	-	expression tag	UNP Q16620
C	1	MET	-	initiating methionine	UNP Q16620
C	2	ALA	-	expression tag	UNP Q16620
C	95	GLN	ASN	engineered mutation	UNP Q16620
C	121	GLN	ASN	engineered mutation	UNP Q16620
C	178	GLN	ASN	engineered mutation	UNP Q16620
C	241	GLN	ASN	conflict	UNP Q16620
C	280	GLN	ASN	engineered mutation	UNP Q16620
C	325	SER	ASN	engineered mutation	UNP Q16620

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Chain	Residue	Modelled	Actual	Comment	Reference
C	384	ALA	-	expression tag	UNP Q16620
C	385	ALA	-	expression tag	UNP Q16620
C	386	ALA	-	expression tag	UNP Q16620
C	387	HIS	-	expression tag	UNP Q16620
C	388	HIS	-	expression tag	UNP Q16620
C	389	HIS	-	expression tag	UNP Q16620
C	390	HIS	-	expression tag	UNP Q16620
C	391	HIS	-	expression tag	UNP Q16620
C	392	HIS	-	expression tag	UNP Q16620

- Molecule 2 is a protein called Neurotrophic factor BDNF precursor form.

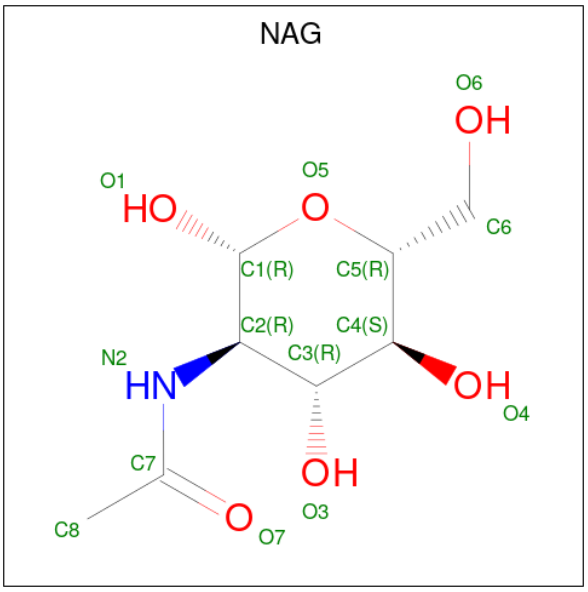
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	116	Total	C	H	N	O	S	0	0	0
			1832	568	916	167	172	9			
2	D	116	Total	C	H	N	O	S	0	0	0
			1832	568	916	167	172	9			

- 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	E	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

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



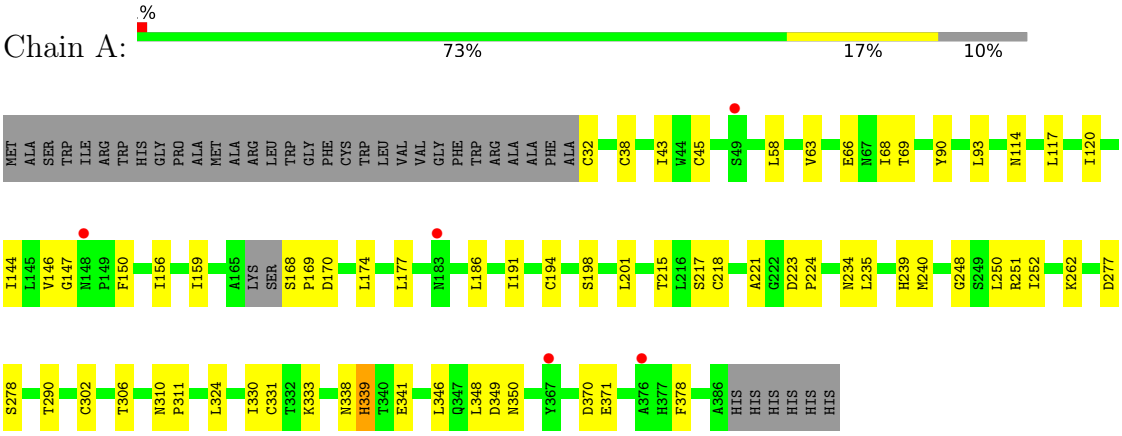
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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.

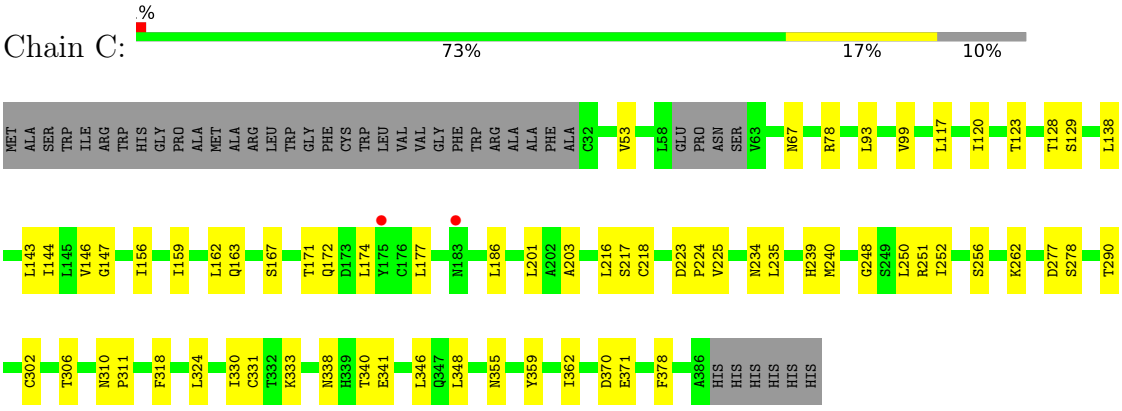
• Molecule 1: BDNF/NT-3 growth factors receptor

Chain A:



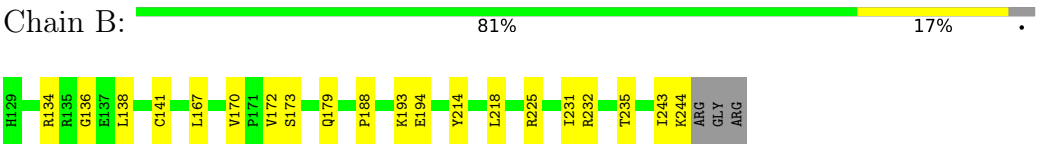
• Molecule 1: BDNF/NT-3 growth factors receptor

Chain C:



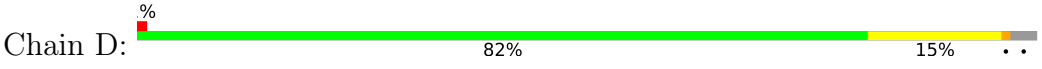
• Molecule 2: Neurotrophic factor BDNF precursor form

Chain B:



• Molecule 2: Neurotrophic factor BDNF precursor form

Chain D:





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

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	56.88Å 179.73Å 183.44Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	64.19 – 3.00 64.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	70.0 (64.19-3.00) 68.9 (64.19-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.253 , 0.285 0.252 , 0.280	Depositor DCC
R_{free} test set	1349 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å^2)	87.1	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 82.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	14646	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.09	0/2812	0.26	0/3828
1	C	0.09	0/2796	0.28	0/3804
2	B	0.11	0/932	0.28	0/1254
2	D	0.10	0/932	0.28	0/1254
All	All	0.09	0/7472	0.27	0/10140

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

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	2747	2661	2660	42	1
1	C	2732	2654	2656	51	0
2	B	916	916	916	14	1
2	D	916	916	916	15	0
3	E	28	25	25	1	0
4	A	28	26	26	2	0
4	C	42	39	39	4	0
All	All	7409	7237	7238	126	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 9.

All (126) 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:117:LEU:HD21	1:C:120:ILE:HD11	1.67	0.76
1:A:117:LEU:HD21	1:A:120:ILE:HD11	1.70	0.73
2:D:214:TYR:OH	2:D:232:ARG:NH2	2.22	0.72
2:B:167:LEU:O	2:B:179:GLN:NE2	2.27	0.68
2:B:214:TYR:OH	2:B:232:ARG:NH2	2.29	0.65
4:C:1102:NAG:C1	4:C:1102:NAG:H82	2.28	0.63
1:C:162:LEU:O	1:C:167:SER:N	2.31	0.62
1:C:171:THR:HG22	1:C:172:GLN:NE2	2.14	0.62
1:A:331:CYS:SG	1:A:333:LYS:NZ	2.74	0.59
1:C:156:ILE:O	1:C:159:ILE:HG22	2.05	0.57
1:A:168:SER:N	1:A:169:PRO:CD	2.68	0.56
1:A:349:ASP:OD1	1:A:350:ASN:ND2	2.39	0.56
4:C:1102:NAG:C1	4:C:1102:NAG:C8	2.84	0.56
1:A:58:LEU:HD13	1:A:63:VAL:HG12	1.88	0.55
1:A:58:LEU:HD22	1:A:63:VAL:HG11	1.89	0.55
1:A:32:CYS:SG	1:A:38:CYS:N	2.79	0.55
1:A:240:MET:SD	1:A:251:ARG:NH2	2.79	0.54
2:D:142:ASP:OD2	2:D:191:TYR:N	2.37	0.54
2:D:142:ASP:OD1	2:D:197:ARG:NH2	2.38	0.54
1:C:235:LEU:HD21	1:C:252:ILE:HD13	1.89	0.53
1:C:146:VAL:HG13	1:C:147:GLY:N	2.23	0.53
1:A:146:VAL:HG13	1:A:147:GLY:N	2.23	0.53
1:C:146:VAL:HG21	1:C:172:GLN:HB2	1.91	0.52
1:A:43:ILE:HD11	1:A:58:LEU:HD21	1.91	0.52
1:C:201:LEU:HD12	1:C:217:SER:O	2.09	0.52
2:D:167:LEU:O	2:D:179:GLN:NE2	2.43	0.52
1:A:201:LEU:HD12	1:A:217:SER:O	2.10	0.52
2:B:231:ILE:HD12	2:B:231:ILE:O	2.10	0.52
2:D:167:LEU:HD12	2:D:218:LEU:CD2	2.40	0.52
2:D:201:LYS:O	2:D:244:LYS:NZ	2.37	0.51
2:D:139:SER:O	2:D:197:ARG:NH1	2.43	0.51
1:C:223:ASP:HB2	1:C:224:PRO:HD3	1.91	0.51
1:A:235:LEU:HD21	1:A:252:ILE:HD13	1.92	0.51
1:C:171:THR:HG22	1:C:172:GLN:CD	2.35	0.51
1:C:338:ASN:HB3	1:C:341:GLU:HB3	1.92	0.50
2:D:194:GLU:OE1	2:D:194:GLU:N	2.39	0.50
1:A:159:ILE:HG23	1:A:186:LEU:HD21	1.94	0.49
1:C:239:HIS:HB3	1:C:252:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:LEU:HD22	1:C:378:PHE:CZ	2.46	0.49
1:A:156:ILE:O	1:A:159:ILE:HG22	2.12	0.49
2:D:231:ILE:O	2:D:231:ILE:HD12	2.13	0.49
1:C:370:ASP:OD1	1:C:371:GLU:N	2.45	0.49
1:C:331:CYS:SG	1:C:333:LYS:NZ	2.85	0.49
1:A:191:ILE:HG23	1:A:194:CYS:O	2.13	0.48
2:B:194:GLU:OE1	2:B:194:GLU:N	2.39	0.48
1:A:348:LEU:HD22	1:A:378:PHE:CZ	2.48	0.48
3:E:1:NAG:C6	3:E:2:NAG:C1	2.91	0.48
1:A:223:ASP:HB2	1:A:224:PRO:HD3	1.95	0.48
1:C:159:ILE:HG23	1:C:186:LEU:HD21	1.95	0.48
1:C:235:LEU:CD2	1:C:252:ILE:HD13	2.44	0.48
2:B:136:GLY:O	2:B:138:LEU:HD12	2.12	0.48
2:B:188:PRO:O	2:B:193:LYS:NZ	2.44	0.48
1:A:370:ASP:OD1	1:A:371:GLU:N	2.47	0.47
1:C:340:THR:O	1:C:340:THR:HG22	2.14	0.47
2:B:167:LEU:HD12	2:B:218:LEU:CD2	2.44	0.47
1:C:338:ASN:O	1:C:338:ASN:OD1	2.32	0.47
1:A:174:LEU:HD12	1:A:174:LEU:N	2.29	0.47
1:A:239:HIS:HB3	1:A:252:ILE:HD12	1.97	0.47
1:A:338:ASN:O	1:A:341:GLU:N	2.34	0.47
1:C:177:LEU:HD23	1:C:177:LEU:H	1.80	0.46
1:A:234:ASN:O	1:A:262:LYS:NZ	2.48	0.46
1:C:99:VAL:HG12	1:C:123:THR:HG22	1.98	0.46
1:A:290:THR:OG1	1:A:306:THR:OG1	2.20	0.46
1:C:146:VAL:HG21	1:C:172:GLN:CB	2.45	0.46
1:C:256:SER:HB2	4:C:1101:NAG:H81	1.98	0.46
1:C:174:LEU:HD12	1:C:174:LEU:N	2.31	0.45
1:C:144:ILE:HD12	1:C:144:ILE:N	2.32	0.45
1:C:355:ASN:O	1:C:359:TYR:OH	2.34	0.45
2:B:172:VAL:HG22	2:B:173:SER:H	1.80	0.45
2:D:208:CYS:SG	2:D:239:CYS:HA	2.56	0.45
4:A:1002:NAG:O7	4:A:1002:NAG:O3	2.33	0.45
1:A:144:ILE:HD12	1:A:144:ILE:N	2.32	0.45
1:C:203:ALA:HB2	1:C:216:LEU:HD22	1.97	0.45
2:D:172:VAL:HG22	2:D:173:SER:H	1.81	0.45
1:C:250:LEU:HD23	1:C:250:LEU:C	2.42	0.44
1:C:290:THR:OG1	1:C:306:THR:OG1	2.19	0.44
1:A:177:LEU:H	1:A:177:LEU:HD23	1.82	0.44
2:B:134:ARG:O	2:B:136:GLY:N	2.46	0.44
2:D:170:VAL:O	2:D:170:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:O	1:A:114:ASN:ND2	2.51	0.44
2:B:170:VAL:HG13	2:B:170:VAL:O	2.17	0.44
1:A:250:LEU:C	1:A:250:LEU:HD23	2.43	0.43
2:D:172:VAL:HG22	2:D:173:SER:N	2.33	0.43
1:A:191:ILE:HD13	1:A:194:CYS:HB3	2.00	0.43
1:A:310:ASN:HB3	1:A:311:PRO:HD3	2.00	0.43
1:C:53:VAL:HG12	1:C:78:ARG:HB3	2.00	0.43
1:C:234:ASN:O	1:C:262:LYS:NZ	2.52	0.43
1:A:277:ASP:OD1	1:A:278:SER:N	2.52	0.43
1:A:43:ILE:HG13	1:A:68:ILE:HD12	2.01	0.43
1:C:218:CYS:O	1:C:248:GLY:N	2.51	0.43
1:A:218:CYS:O	1:A:248:GLY:N	2.52	0.43
1:A:346:LEU:O	1:A:348:LEU:HD12	2.18	0.43
2:B:172:VAL:HG22	2:B:173:SER:N	2.34	0.43
1:C:143:LEU:O	1:C:167:SER:O	2.37	0.43
1:C:310:ASN:HB3	1:C:311:PRO:HD3	2.01	0.43
1:A:66:GLU:HB2	4:A:1001:NAG:O7	2.18	0.42
1:A:93:LEU:C	1:A:93:LEU:HD23	2.43	0.42
1:C:99:VAL:HG12	1:C:123:THR:CG2	2.49	0.42
1:C:93:LEU:C	1:C:93:LEU:HD23	2.44	0.42
1:C:277:ASP:OD1	1:C:278:SER:N	2.53	0.42
1:C:346:LEU:O	1:C:348:LEU:HD12	2.19	0.42
2:B:218:LEU:HD23	2:B:218:LEU:C	2.45	0.42
1:C:240:MET:SD	1:C:251:ARG:NH2	2.93	0.42
1:C:318:PHE:CE1	1:C:362:ILE:HD12	2.55	0.42
1:A:150:PHE:O	1:A:177:LEU:HD23	2.20	0.41
2:B:235:THR:HG22	2:B:235:THR:O	2.20	0.41
1:C:201:LEU:HD11	1:C:216:LEU:HB3	2.01	0.41
1:C:163:GLN:HA	1:C:167:SER:CB	2.49	0.41
2:D:235:THR:HG22	2:D:235:THR:O	2.21	0.41
1:A:324:LEU:HD21	1:A:330:ILE:HG21	2.03	0.41
1:A:69:THR:O	1:A:69:THR:HG22	2.19	0.41
1:C:163:GLN:HA	1:C:167:SER:HB3	2.03	0.41
1:C:225:VAL:O	1:C:225:VAL:HG13	2.21	0.41
1:C:252:ILE:O	1:C:252:ILE:HG23	2.21	0.41
2:D:218:LEU:HD23	2:D:218:LEU:C	2.46	0.41
1:A:198:SER:N	1:A:221:ALA:O	2.50	0.40
1:A:215:THR:HG22	1:A:251:ARG:HG3	2.03	0.40
1:A:338:ASN:O	1:A:339:HIS:C	2.64	0.40
1:C:117:LEU:HD23	1:C:138:LEU:HD13	2.03	0.40
1:C:171:THR:HG22	1:C:172:GLN:HE22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:LEU:HD21	1:C:330:ILE:HG21	2.03	0.40
1:C:338:ASN:HB3	1:C:341:GLU:O	2.20	0.40
1:A:252:ILE:O	1:A:252:ILE:HG23	2.21	0.40
1:C:67:ASN:HD21	4:C:1102:NAG:C1	2.35	0.40
1:C:128:THR:O	1:C:129:SER:OG	2.37	0.40
2:B:243:ILE:O	2:B:244:LYS:HB3	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:170:ASP:O	2:B:225:ARG:NH1[3_445]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	349/392 (89%)	324 (93%)	24 (7%)	1 (0%)	36 70
1	C	347/392 (88%)	321 (92%)	26 (8%)	0	100 100
2	B	114/119 (96%)	107 (94%)	7 (6%)	0	100 100
2	D	114/119 (96%)	106 (93%)	8 (7%)	0	100 100
All	All	924/1022 (90%)	858 (93%)	65 (7%)	1 (0%)	48 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	HIS

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	314/344 (91%)	312 (99%)	2 (1%)	78 88
1	C	312/344 (91%)	311 (100%)	1 (0%)	86 91
2	B	103/105 (98%)	102 (99%)	1 (1%)	68 84
2	D	103/105 (98%)	102 (99%)	1 (1%)	68 84
All	All	832/898 (93%)	827 (99%)	5 (1%)	78 88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	CYS
1	A	302	CYS
2	B	141	CYS
1	C	302	CYS
2	D	208	CYS

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	95	GLN
1	A	114	ASN
1	A	119	HIS
1	A	137	HIS
1	C	119	HIS
1	C	338	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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.68	1 (7%)	17,19,21	0.82	0
3	NAG	E	2	3	14,14,15	0.35	0	17,19,21	0.49	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	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.43	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C3-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6

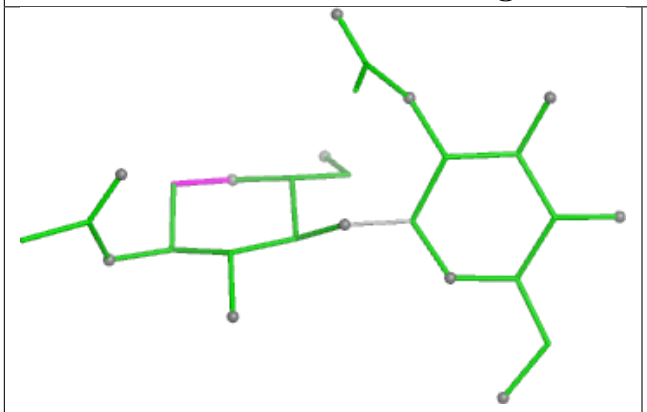
There are no ring outliers.

2 monomers are involved in 1 short contact:

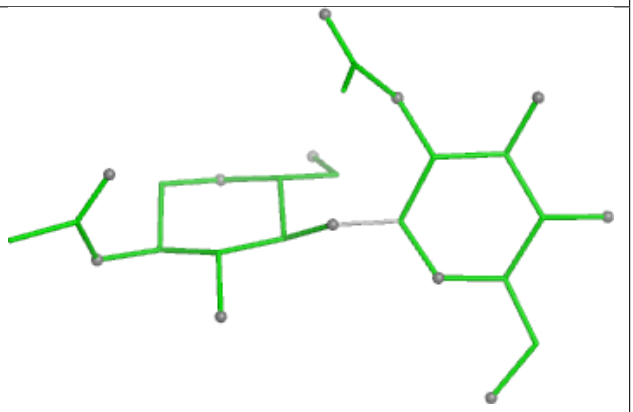
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
3	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

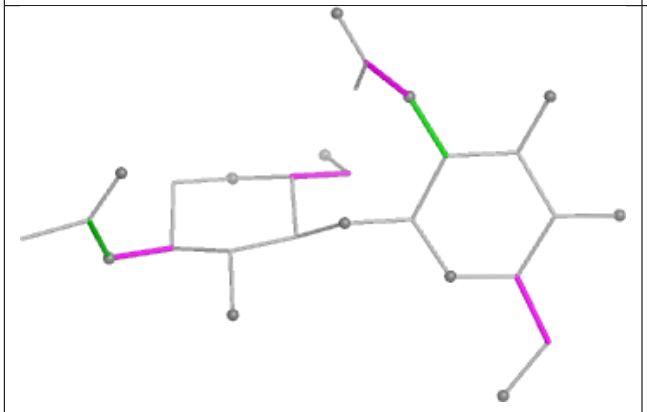
Oligosaccharide Chain E



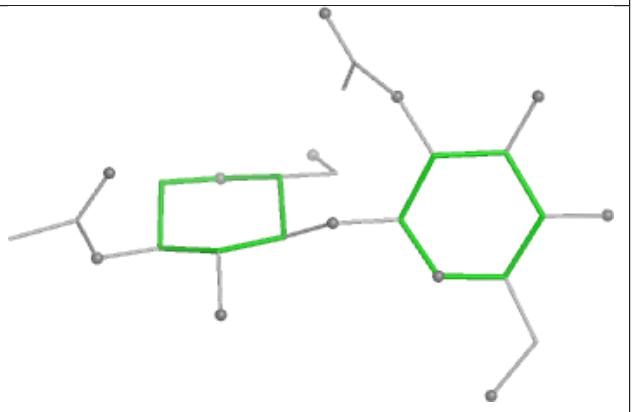
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

5 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	NAG	C	1102	-	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
4	NAG	A	1002	1	14,14,15	0.21	0	17,19,21	0.49	0
4	NAG	C	1101	1	14,14,15	0.21	0	17,19,21	0.31	0
4	NAG	A	1001	1	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	C	1103	-	14,14,15	0.58	1 (7%)	17,19,21	0.54	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	NAG	C	1102	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1101	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1103	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1103	NAG	O5-C1	-2.05	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1102	NAG	C2-N2-C7	2.72	126.78	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	C4-C5-C6-O6
4	C	1101	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	A	1001	NAG	C8-C7-N2-C2
4	A	1001	NAG	O7-C7-N2-C2
4	C	1102	NAG	C8-C7-N2-C2
4	C	1102	NAG	O7-C7-N2-C2
4	C	1101	NAG	C4-C5-C6-O6
4	A	1002	NAG	O5-C5-C6-O6
4	C	1102	NAG	C1-C2-N2-C7
4	A	1002	NAG	C1-C2-N2-C7
4	C	1101	NAG	C1-C2-N2-C7
4	A	1002	NAG	C3-C2-N2-C7
4	C	1101	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1102	NAG	3	0
4	A	1002	NAG	1	0
4	C	1101	NAG	1	0
4	A	1001	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	353/392 (90%)	-0.33	5 (1%)	73	51	81, 126, 187, 225	0
1	C	351/392 (89%)	-0.35	2 (0%)	85	69	75, 128, 179, 232	0
2	B	116/119 (97%)	-0.33	0	100	100	60, 113, 158, 184	0
2	D	116/119 (97%)	-0.31	1 (0%)	81	61	60, 114, 175, 193	0
All	All	936/1022 (91%)	-0.34	8 (0%)	81	61	60, 123, 180, 232	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	SER	4.6
1	A	183	ASN	3.4
1	A	376	ALA	2.9
1	C	183	ASN	2.6
1	C	175	TYR	2.5
2	D	156	ALA	2.2
1	A	367	TYR	2.1
1	A	148	ASN	2.0

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

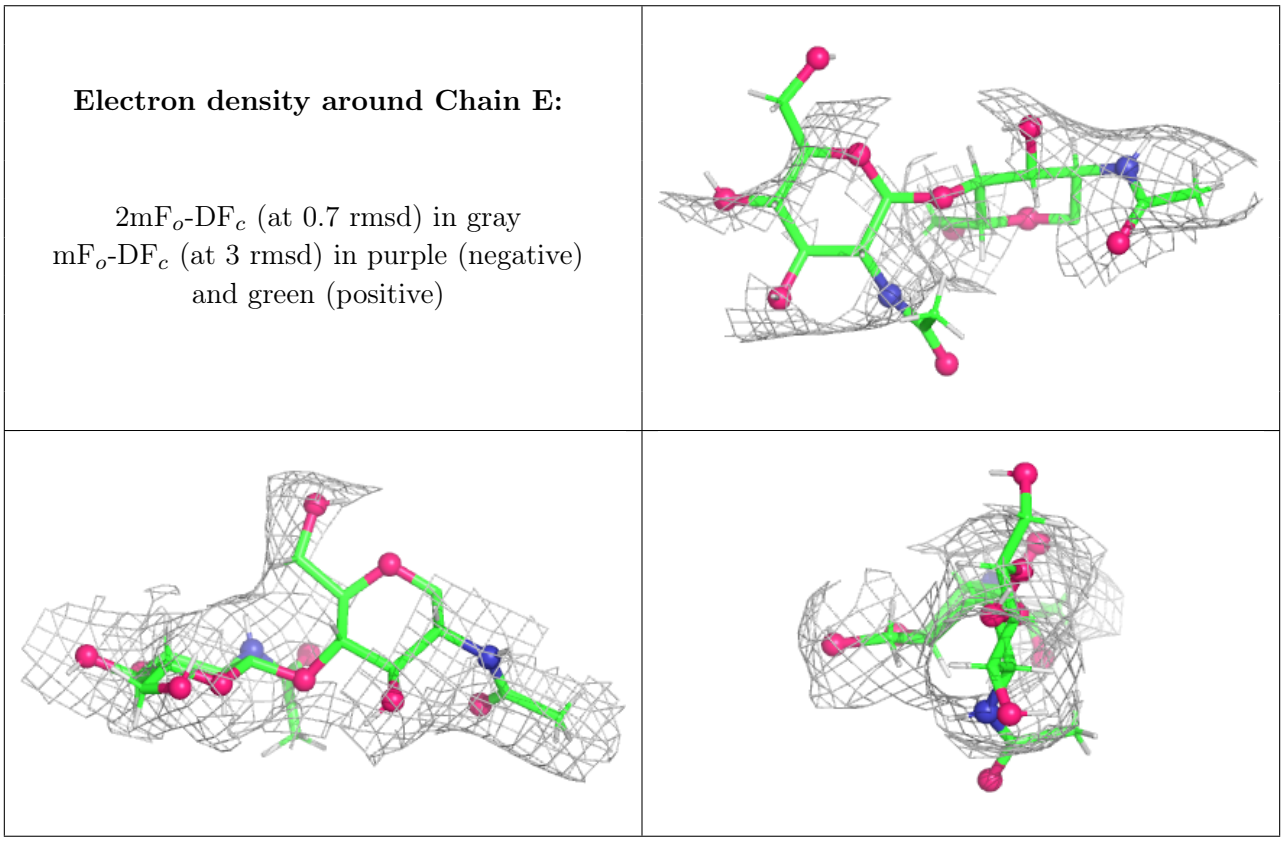
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	1	14/15	0.95	0.07	123,161,197,203	0
3	NAG	E	2	14/15	0.96	0.11	168,181,218,219	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(Å^2)	Q<0.9
4	NAG	C	1102	14/15	0.91	0.09	139,163,195,198	0
4	NAG	A	1001	14/15	0.94	0.07	153,166,197,201	0
4	NAG	A	1002	14/15	0.95	0.08	132,165,207,208	0
4	NAG	C	1101	14/15	0.96	0.06	137,159,190,199	0
4	NAG	C	1103	14/15	0.97	0.10	141,158,189,190	0

6.5 Other polymers (i)

There are no such residues in this entry.