Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2025 – 08:32 PM EDT

PDB ID	:	4DW0 / pdb_00004dw0
Title	:	Crystal structure of the ATP-gated P2X4 ion channel in the closed, apo state at 2.9 Angstroms
Authors	:	Hattori, M.; Gouaux, E.
Deposited on	:	2012-02-24
Resolution	:	2.90 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:

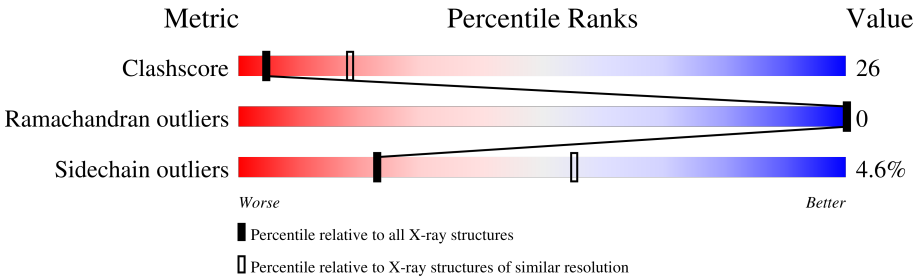
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.90 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))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	340	57% 38%
2	B	4	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	507	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2670 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 P2X purinoceptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2502	1584	426	476	16	0	0	0

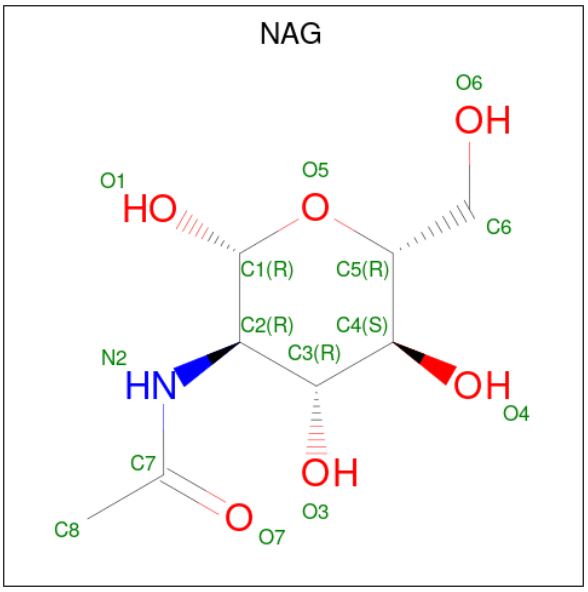
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP Q6NYR1
A	27	SER	-	expression tag	UNP Q6NYR1
A	51	PHE	CYS	engineered mutation	UNP Q6NYR1
A	78	LYS	ASN	engineered mutation	UNP Q6NYR1
A	187	ARG	ASN	engineered mutation	UNP Q6NYR1
A	252	ARG	HIS	engineered mutation	UNP Q6NYR1

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

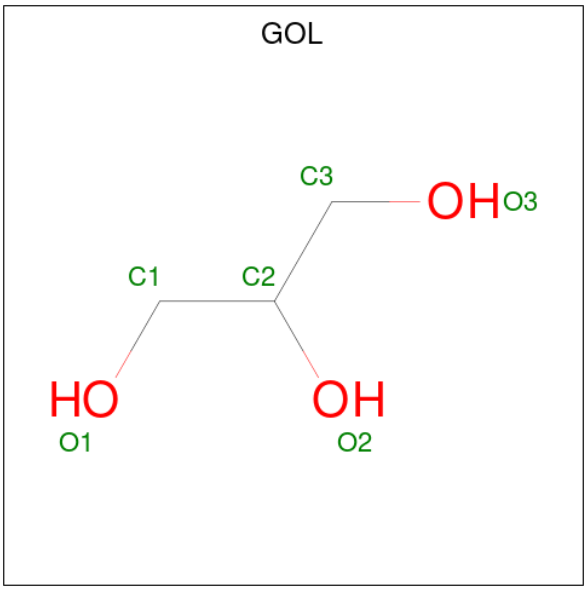


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Gd	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	79	Total O 79 79	0	0

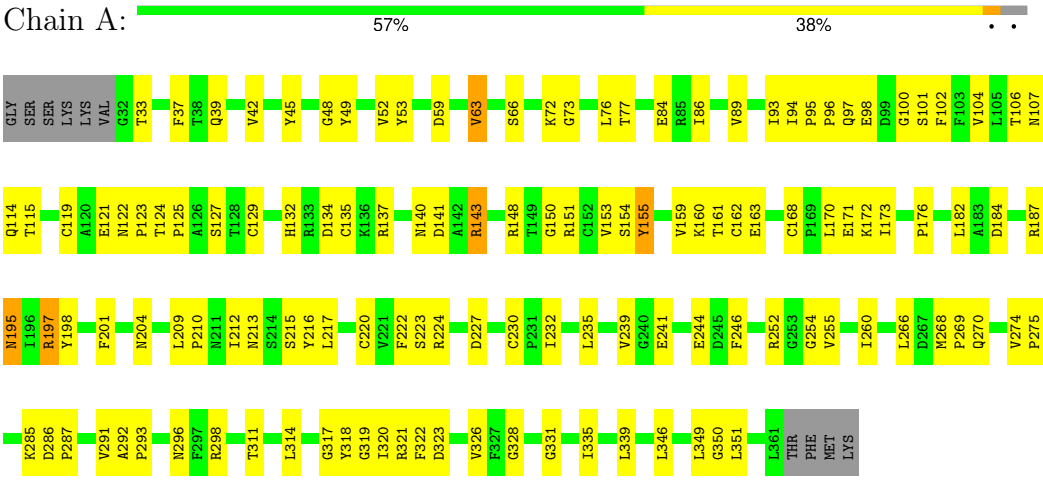
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: P2X purinoceptor

Chain A:



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

Chain B:

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	99.63Å 99.63Å 441.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.18 – 2.90	Depositor
% Data completeness (in resolution range)	97.1 (47.18-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.220 , 0.244	Depositor
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.825	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2670	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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: BMA, GD, MAN, GOL, 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	0.44	0/2558	0.64	0/3488

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	2502	0	2352	126	0
2	B	50	0	43	3	0
3	A	14	0	13	0	0
4	A	1	0	0	0	0
5	A	24	0	32	10	0
6	A	79	0	0	5	0
All	All	2670	0	2440	129	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 26.

All (129) 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:98:GLU:O	5:A:510:GOL:H2	1.62	0.97
1:A:241:GLU:HG2	1:A:279:PHE:CD2	2.16	0.81
1:A:212:ILE:HD12	1:A:212:ILE:H	1.45	0.80
1:A:184:ASP:O	1:A:187:ARG:HG2	1.83	0.79
2:B:2:NAG:H83	2:B:4:MAN:O2	1.84	0.78
1:A:124:THR:HG22	1:A:125:PRO:HD2	1.67	0.76
1:A:124:THR:H	1:A:127:SER:HB2	1.50	0.76
1:A:115:THR:HG22	1:A:311:THR:HG22	1.69	0.74
1:A:123:PRO:HD3	1:A:155:TYR:CE1	2.23	0.73
1:A:100:GLY:N	5:A:510:GOL:O2	2.20	0.69
1:A:137:ARG:HB2	1:A:150:GLY:H	1.59	0.67
1:A:154:SER:HA	1:A:160:LYS:HA	1.77	0.67
1:A:254:GLY:O	1:A:320:ILE:HA	1.95	0.67
1:A:159:VAL:HG12	1:A:160:LYS:H	1.60	0.66
1:A:73:GLY:H	5:A:508:GOL:H31	1.62	0.64
1:A:346:LEU:O	1:A:349:LEU:HG	1.96	0.64
1:A:217:LEU:HD23	1:A:217:LEU:N	2.14	0.63
1:A:349:LEU:HD12	1:A:350:GLY:N	2.14	0.63
1:A:76:LEU:HD12	1:A:77:THR:N	2.14	0.62
1:A:45:TYR:O	1:A:49:TYR:HB3	1.99	0.62
1:A:223:SER:HB3	1:A:227:ASP:H	1.66	0.61
1:A:76:LEU:HD12	1:A:77:THR:H	1.66	0.60
1:A:216:TYR:O	1:A:220:CYS:HB2	2.01	0.59
1:A:212:ILE:H	1:A:212:ILE:CD1	2.15	0.59
1:A:59:ASP:O	1:A:331:GLY:HA2	2.01	0.59
1:A:201:PHE:CD2	1:A:266:LEU:HD12	2.38	0.59
1:A:239:VAL:HG21	1:A:246:PHE:HD1	1.68	0.59
1:A:106:THR:O	1:A:182:LEU:HB2	2.03	0.58
1:A:124:THR:N	1:A:127:SER:HB2	2.18	0.58
1:A:121:GLU:O	1:A:161:THR:HG21	2.04	0.58
1:A:239:VAL:HG21	1:A:246:PHE:CD1	2.39	0.58
2:B:2:NAG:H3	2:B:3:BMA:H2	1.86	0.57
1:A:89:VAL:HG23	5:A:508:GOL:O1	2.04	0.57
1:A:132:HIS:CD2	1:A:151:ARG:HA	2.39	0.57
1:A:172:LYS:HG2	6:A:658:HOH:O	2.04	0.57
1:A:119:CYS:SG	1:A:170:LEU:HD22	2.46	0.56
1:A:255:VAL:HG12	1:A:282:LEU:HD12	1.87	0.55
1:A:204:ASN:HB3	6:A:647:HOH:O	2.07	0.55
1:A:212:ILE:HD12	1:A:212:ILE:N	2.19	0.55
1:A:244:GLU:OE1	1:A:285:LYS:HE3	2.06	0.55
1:A:260:ILE:HB	1:A:326:VAL:HG22	1.87	0.55
1:A:63:VAL:HB	1:A:328:GLY:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HB2	1:A:150:GLY:N	2.22	0.55
1:A:188:PHE:HB2	1:A:235:LEU:HD12	1.90	0.54
1:A:66:SER:HA	6:A:678:HOH:O	2.07	0.54
1:A:93:ILE:C	1:A:94:ILE:HG13	2.28	0.54
1:A:106:THR:OG1	1:A:319:GLY:HA2	2.08	0.54
1:A:123:PRO:HD3	1:A:155:TYR:HE1	1.69	0.53
1:A:201:PHE:HD2	1:A:266:LEU:HD12	1.72	0.53
1:A:115:THR:CG2	1:A:311:THR:HG22	2.38	0.53
2:B:2:NAG:H3	2:B:3:BMA:C2	2.39	0.53
1:A:212:ILE:CG2	1:A:217:LEU:HD11	2.39	0.53
1:A:108:MET:HG3	1:A:110:ILE:HG13	1.91	0.52
1:A:159:VAL:HG12	1:A:160:LYS:N	2.23	0.52
1:A:73:GLY:H	5:A:508:GOL:C3	2.22	0.52
1:A:190:VAL:O	1:A:190:VAL:HG13	2.10	0.51
1:A:296:ASN:HA	1:A:317:GLY:O	2.10	0.51
1:A:212:ILE:HG23	1:A:216:TYR:HD2	1.75	0.51
1:A:108:MET:HG3	1:A:110:ILE:CG1	2.41	0.51
1:A:292:ALA:N	1:A:293:PRO:HD3	2.26	0.51
1:A:298:ARG:HD3	1:A:314:LEU:HD21	1.91	0.51
1:A:195:ASN:HB3	5:A:507:GOL:C1	2.42	0.50
1:A:268:MET:HB3	1:A:269:PRO:HD2	1.94	0.50
1:A:93:ILE:O	1:A:94:ILE:HG13	2.12	0.50
1:A:241:GLU:HG2	1:A:279:PHE:HD2	1.72	0.50
1:A:322:PHE:N	1:A:322:PHE:CD1	2.80	0.50
1:A:108:MET:HE1	1:A:182:LEU:HD13	1.94	0.50
1:A:296:ASN:HB3	1:A:318:TYR:CD1	2.47	0.49
1:A:268:MET:HB3	1:A:269:PRO:CD	2.43	0.49
1:A:114:GLN:HA	1:A:168:CYS:O	2.13	0.49
1:A:153:VAL:HG22	1:A:163:GLU:HB2	1.94	0.49
1:A:155:TYR:CD2	1:A:155:TYR:C	2.85	0.49
1:A:66:SER:HB3	5:A:507:GOL:O1	2.13	0.49
1:A:48:GLY:HA2	1:A:52:VAL:HG22	1.95	0.49
1:A:335:ILE:O	1:A:339:LEU:HG	2.13	0.49
1:A:209:LEU:HB3	1:A:210:PRO:HD2	1.94	0.48
1:A:33:THR:O	1:A:37:PHE:HB3	2.13	0.48
1:A:212:ILE:HG21	1:A:217:LEU:HD11	1.93	0.48
1:A:135:CYS:HB2	1:A:150:GLY:O	2.14	0.48
1:A:137:ARG:HA	1:A:148:ARG:O	2.13	0.48
1:A:119:CYS:SG	1:A:170:LEU:CD2	3.03	0.47
1:A:72:LYS:HE2	1:A:189:THR:OG1	2.14	0.47
1:A:222:PHE:HA	1:A:230:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASP:OD1	1:A:287:PRO:HD2	2.14	0.47
1:A:98:GLU:HB2	1:A:101:SER:O	2.14	0.47
1:A:148:ARG:NH1	1:A:162:CYS:SG	2.88	0.47
1:A:95:PRO:HB2	1:A:96:PRO:CD	2.45	0.46
1:A:49:TYR:O	1:A:53:TYR:HB3	2.16	0.46
1:A:222:PHE:HB2	1:A:230:CYS:O	2.16	0.46
1:A:73:GLY:HA2	5:A:509:GOL:H2	1.96	0.46
1:A:122:ASN:O	1:A:127:SER:CB	2.64	0.46
1:A:171:GLU:OE1	1:A:298:ARG:NH1	2.48	0.46
1:A:209:LEU:HB2	1:A:212:ILE:HD13	1.97	0.46
1:A:195:ASN:HB3	5:A:507:GOL:O1	2.16	0.46
1:A:124:THR:O	1:A:125:PRO:C	2.52	0.46
1:A:155:TYR:HB2	1:A:161:THR:HG22	1.97	0.46
1:A:72:LYS:NZ	1:A:232:ILE:HD13	2.31	0.46
1:A:97:GLN:HA	6:A:671:HOH:O	2.16	0.46
1:A:72:LYS:HE2	1:A:72:LYS:HB2	1.70	0.45
1:A:239:VAL:HG11	1:A:246:PHE:N	2.31	0.45
1:A:63:VAL:HG23	1:A:198:TYR:CE2	2.51	0.45
1:A:176:PRO:HB3	1:A:318:TYR:CE2	2.51	0.45
1:A:102:PHE:CZ	1:A:190:VAL:HG21	2.52	0.45
1:A:129:CYS:HB2	1:A:134:ASP:HB2	1.99	0.45
1:A:195:ASN:HB3	5:A:507:GOL:H12	1.98	0.45
1:A:143:ARG:HD3	1:A:173:ILE:HD11	1.98	0.44
1:A:215:SER:N	6:A:661:HOH:O	2.50	0.44
1:A:351:LEU:O	1:A:351:LEU:HD13	2.17	0.43
1:A:104:VAL:O	1:A:319:GLY:HA3	2.18	0.43
1:A:216:TYR:C	1:A:217:LEU:HD23	2.39	0.43
1:A:239:VAL:CG2	1:A:246:PHE:HD1	2.31	0.43
1:A:107:ASN:ND2	1:A:176:PRO:HB2	2.34	0.42
1:A:171:GLU:OE2	1:A:298:ARG:NH1	2.51	0.42
1:A:216:TYR:CD2	1:A:217:LEU:HD21	2.54	0.42
1:A:123:PRO:HG3	1:A:155:TYR:HD1	1.85	0.42
1:A:176:PRO:HD2	1:A:252:ARG:NH2	2.34	0.42
1:A:244:GLU:OE1	1:A:285:LYS:CE	2.67	0.42
1:A:197:ARG:HB2	1:A:204:ASN:OD1	2.20	0.42
1:A:224:ARG:HA	1:A:224:ARG:HD3	1.91	0.42
1:A:143:ARG:NH2	1:A:171:GLU:O	2.53	0.41
1:A:216:TYR:O	1:A:220:CYS:N	2.53	0.41
1:A:321:ARG:NH1	1:A:323:ASP:OD2	2.53	0.41
1:A:155:TYR:O	1:A:155:TYR:HD2	2.02	0.41
1:A:197:ARG:HB2	1:A:197:ARG:HE	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:O	1:A:42:VAL:HG22	2.20	0.41
1:A:274:VAL:HB	1:A:275:PRO:HD2	2.03	0.41
1:A:320:ILE:O	1:A:322:PHE:CE1	2.73	0.41
1:A:255:VAL:CG1	1:A:282:LEU:HD12	2.50	0.41
1:A:86:ILE:HD13	1:A:86:ILE:HA	1.78	0.41

There are no symmetry-related clashes.

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	328/340 (96%)	315 (96%)	13 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	262/298 (88%)	250 (95%)	12 (5%)	23 55

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL

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Mol	Chain	Res	Type
1	A	84	GLU
1	A	108	MET
1	A	140	ASN
1	A	141	ASP
1	A	143	ARG
1	A	155	TYR
1	A	195	ASN
1	A	197	ARG
1	A	213	ASN
1	A	270	GLN
1	A	291	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
2	NAG	B	1	2,1	14,14,15	0.65	0	17,19,21	1.34	3 (17%)
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	1.25	2 (11%)
2	BMA	B	3	2	11,11,12	0.48	0	15,15,17	1.31	1 (6%)
2	MAN	B	4	2	11,11,12	0.63	0	15,15,17	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C2-N2-C7	-3.45	118.28	122.90
2	B	3	BMA	C1-O5-C5	3.04	116.26	112.19
2	B	1	NAG	C2-N2-C7	-2.89	119.03	122.90
2	B	1	NAG	C4-C3-C2	2.78	115.09	111.02
2	B	2	NAG	C1-O5-C5	2.51	115.55	112.19
2	B	1	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

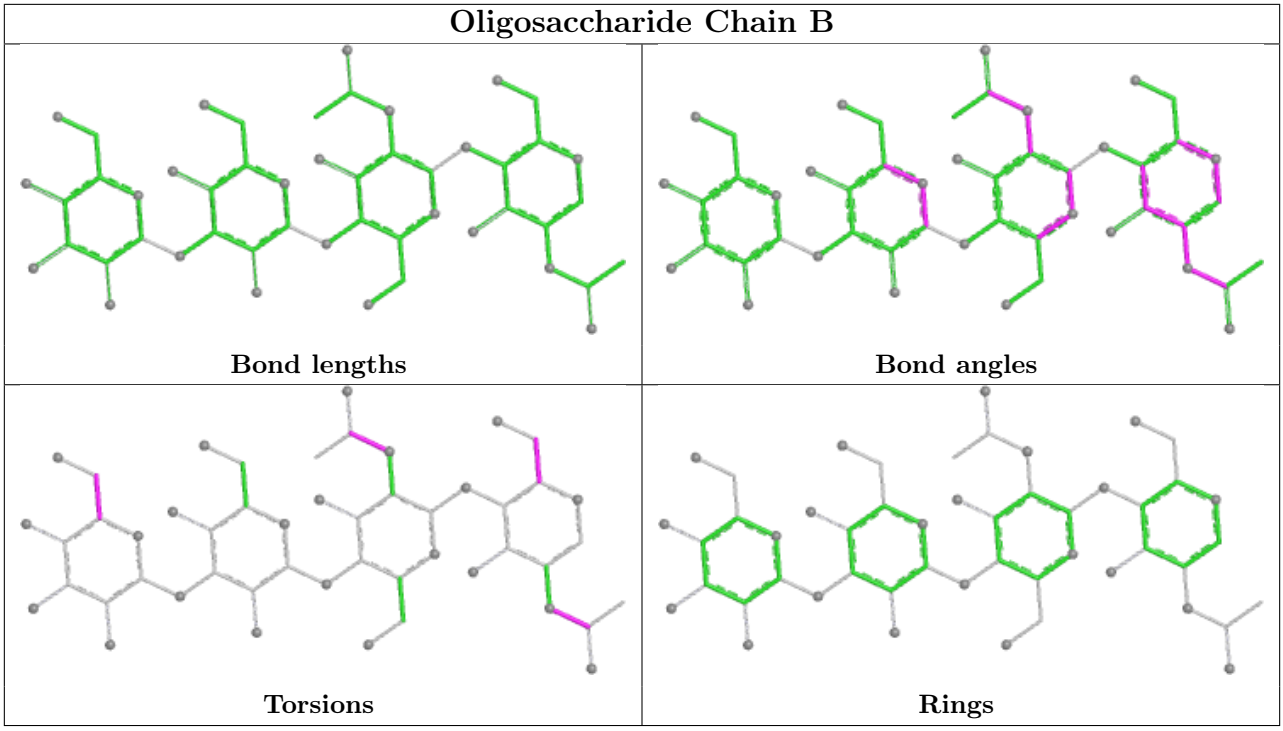
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	4	MAN	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	3	0
2	B	4	MAN	1	0
2	B	3	BMA	2	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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	GOL	A	510	-	5,5,5	0.40	0	5,5,5	1.16	1 (20%)
5	GOL	A	508	-	5,5,5	0.35	0	5,5,5	0.28	0
3	NAG	A	505	1	14,14,15	0.72	0	17,19,21	2.11	6 (35%)
5	GOL	A	507	-	5,5,5	0.33	0	5,5,5	0.77	0
5	GOL	A	509	-	5,5,5	0.41	0	5,5,5	0.45	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
5	GOL	A	510	-	-	4/4/4/4	-
5	GOL	A	508	-	-	4/4/4/4	-
3	NAG	A	505	1	-	0/6/23/26	0/1/1/1
5	GOL	A	507	-	-	0/4/4/4	-
5	GOL	A	509	-	-	4/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	505	NAG	O5-C5-C6	4.46	116.34	107.66
3	A	505	NAG	C2-N2-C7	-3.85	117.75	122.90
3	A	505	NAG	C1-O5-C5	-3.78	107.13	112.19
3	A	505	NAG	C8-C7-N2	2.78	120.72	116.12
3	A	505	NAG	O5-C5-C4	-2.18	105.52	110.83
5	A	510	GOL	O2-C2-C1	2.16	118.11	109.18
3	A	505	NAG	O7-C7-C8	-2.06	118.39	122.05

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	GOL	O1-C1-C2-C3
5	A	509	GOL	O1-C1-C2-C3
5	A	510	GOL	O1-C1-C2-C3
5	A	508	GOL	C1-C2-C3-O3
5	A	509	GOL	C1-C2-C3-O3
5	A	508	GOL	O1-C1-C2-O2
5	A	508	GOL	O2-C2-C3-O3
5	A	509	GOL	O2-C2-C3-O3
5	A	510	GOL	O2-C2-C3-O3
5	A	510	GOL	O1-C1-C2-O2
5	A	509	GOL	O1-C1-C2-O2
5	A	510	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	510	GOL	2	0
5	A	508	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	GOL	4	0
5	A	509	GOL	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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

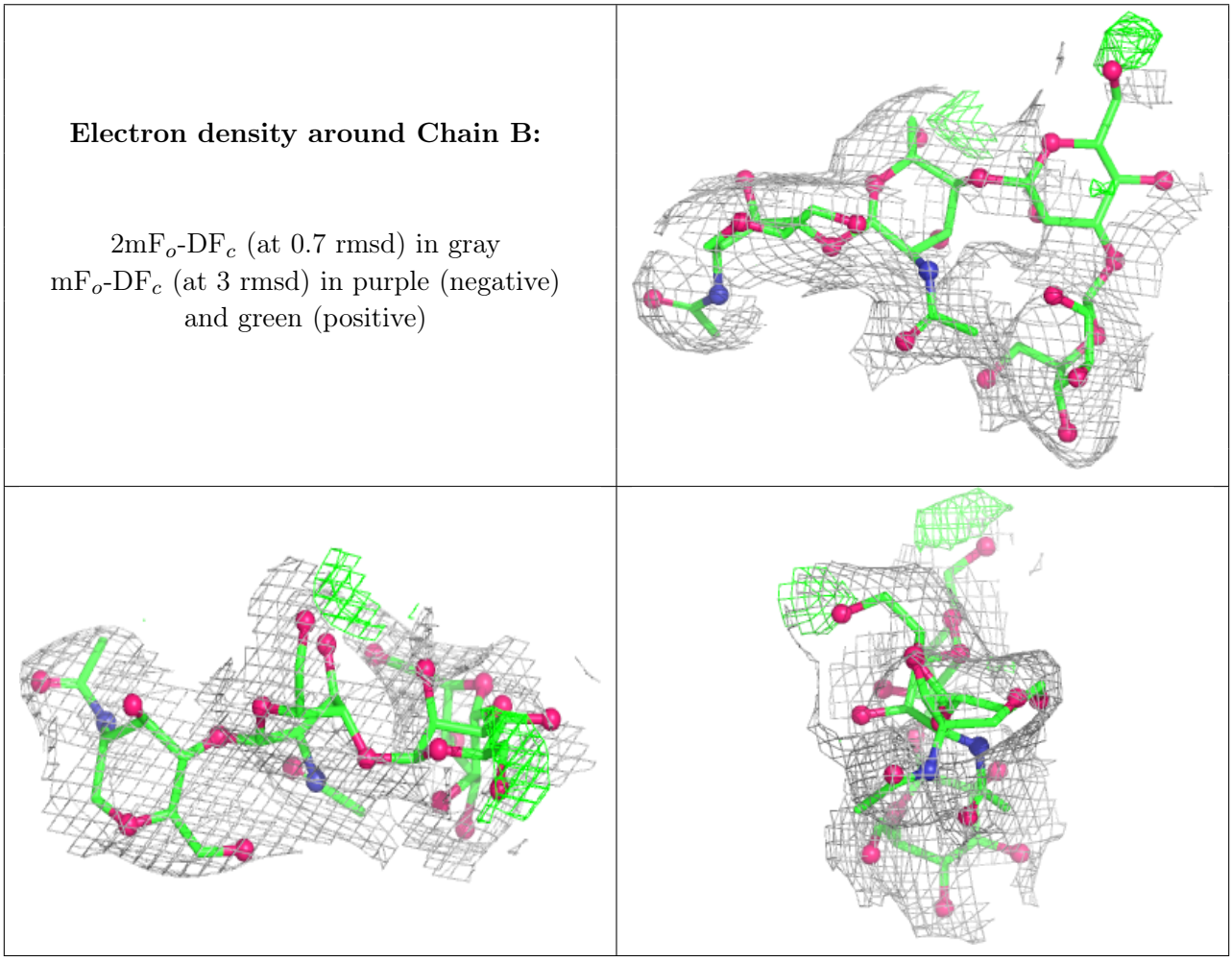
6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

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.

Electron density around Chain B:

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



6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.