



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:04 PM UTC

PDB ID : 4M4P / pdb_00004m4p
Title : Crystal structure of EPHA4 ectodomain
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Deposited on : 2013-08-07
Resolution : 2.08 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

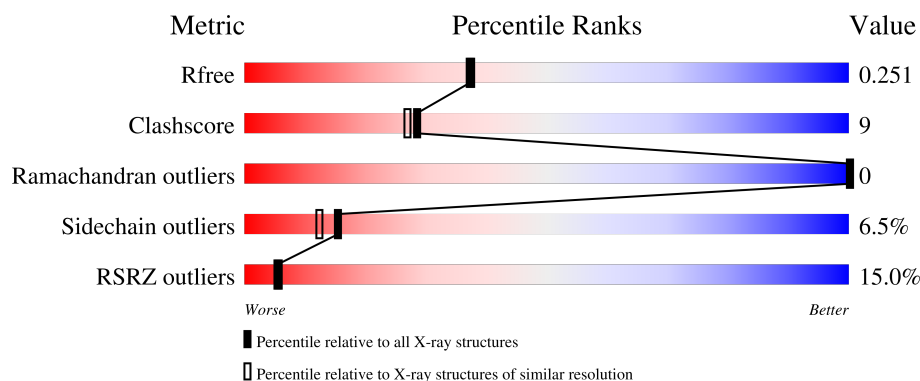
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	518	15% 78% 18% ..
2	B	2	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
3	NAG	A	601	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4214 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 Ephrin type-A receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3997	2493	691	787	26			

There is a discrepancy between the modelled and reference sequences:

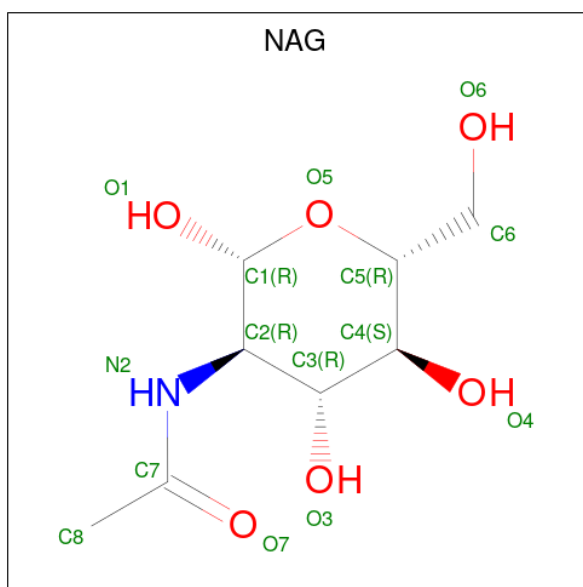
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	expression tag	UNP P54764

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

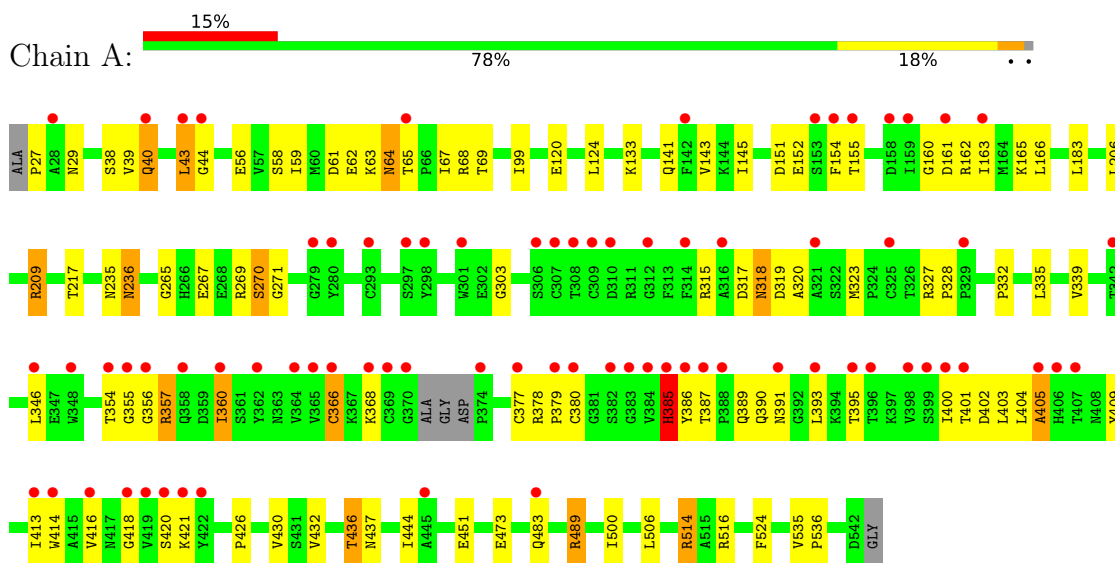
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		

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: Ephrin type-A receptor 4



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	112.59Å 112.59Å 49.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.00 – 2.08 27.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.00-2.08) 97.1 (27.00-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.189 , 0.225 (Not available) , 0.251	Depositor DCC
R_{free} test set	1981 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l 0.039 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4214	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

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	0.55	0/4082	0.93	7/5552 (0.1%)

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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	GLY	N-CA-C	11.20	128.02	114.69
1	A	405	ALA	N-CA-C	9.02	121.04	111.03
1	A	421	LYS	N-CA-C	-5.95	105.51	112.89
1	A	500	ILE	CB-CA-C	-5.40	104.42	110.96
1	A	385	HIS	CA-C-N	5.33	131.30	121.70
1	A	385	HIS	C-N-CA	5.33	131.30	121.70
1	A	133	LYS	N-CA-C	5.10	118.81	112.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	LEU	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	3997	0	3856	70	0
2	B	28	0	25	0	0
3	A	28	0	26	0	0
4	A	161	0	0	8	0
All	All	4214	0	3907	70	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 9.

All (70) 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:385:HIS:HA	1:A:386:TYR:HB2	1.51	0.91
1:A:270:SER:OG	1:A:271:GLY:N	2.04	0.87
1:A:451:GLU:OE2	4:A:780:HOH:O	2.01	0.76
1:A:405:ALA:HB1	1:A:437:ASN:HD21	1.50	0.75
1:A:390:GLN:O	1:A:391:ASN:ND2	2.20	0.73
1:A:444:ILE:O	4:A:800:HOH:O	2.08	0.69
1:A:58:SER:OG	1:A:68:ARG:NH2	2.26	0.68
1:A:270:SER:HG	1:A:271:GLY:H	1.38	0.64
1:A:270:SER:HG	1:A:271:GLY:N	1.93	0.62
1:A:386:TYR:CD1	1:A:390:GLN:HG3	2.36	0.59
1:A:38:SER:O	1:A:40:GLN:NE2	2.35	0.59
1:A:236:ASN:OD1	1:A:236:ASN:N	2.37	0.58
1:A:473:GLU:OE1	1:A:516:ARG:NH1	2.36	0.58
1:A:335:LEU:CD1	1:A:346:LEU:HD21	2.34	0.57
1:A:335:LEU:HD22	1:A:430:VAL:HG13	1.86	0.56
1:A:405:ALA:HB1	1:A:437:ASN:ND2	2.21	0.56
1:A:39:VAL:HA	4:A:848:HOH:O	2.07	0.55
1:A:61:ASP:HA	1:A:161:ASP:HA	1.88	0.55
1:A:405:ALA:O	1:A:436:THR:HB	2.07	0.54
1:A:64:ASN:OD1	1:A:64:ASN:N	2.38	0.53
1:A:320:ALA:HB3	1:A:323:MET:HG3	1.90	0.53
1:A:62:GLU:N	1:A:160:GLY:O	2.31	0.53
1:A:267:GLU:OE2	1:A:269:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HD12	1:A:69:THR:HG21	1.92	0.52
1:A:155:THR:OG1	1:A:165:LYS:HG3	2.11	0.51
1:A:217:THR:OG1	4:A:798:HOH:O	2.19	0.51
1:A:385:HIS:O	1:A:401:THR:OG1	2.26	0.51
1:A:378:ARG:HB3	1:A:379:PRO:HD2	1.92	0.51
1:A:386:TYR:HB3	1:A:390:GLN:HB2	1.93	0.51
1:A:368:LYS:O	1:A:377:CYS:HA	2.12	0.49
1:A:265:GLY:O	1:A:303:GLY:HA2	2.13	0.49
1:A:386:TYR:H	1:A:400:ILE:HA	1.77	0.49
1:A:61:ASP:O	1:A:162:ARG:NH1	2.44	0.48
1:A:378:ARG:HB3	1:A:379:PRO:CD	2.43	0.48
1:A:328:PRO:HB3	1:A:420:SER:CB	2.42	0.48
1:A:354:THR:C	1:A:356:GLY:HA2	2.38	0.47
1:A:386:TYR:CE1	1:A:390:GLN:HG3	2.50	0.47
1:A:368:LYS:HE3	1:A:380:CYS:HB2	1.96	0.47
1:A:27:PRO:HB2	1:A:29:ASN:OD1	2.13	0.47
1:A:414:TRP:CH2	1:A:426:PRO:HA	2.49	0.47
1:A:319:ASP:OD1	1:A:320:ALA:N	2.48	0.47
1:A:163:ILE:HG21	1:A:166:LEU:HD13	1.98	0.46
1:A:354:THR:HG23	1:A:356:GLY:HA3	1.98	0.46
1:A:366:CYS:HB3	1:A:386:TYR:OH	2.16	0.45
1:A:56:GLU:HG2	4:A:811:HOH:O	2.15	0.45
1:A:124:LEU:HG	1:A:145:ILE:HD12	1.98	0.44
1:A:318:ASN:N	1:A:318:ASN:OD1	2.49	0.44
1:A:386:TYR:CG	1:A:390:GLN:HG3	2.52	0.44
1:A:141:GLN:O	4:A:814:HOH:O	2.21	0.43
1:A:209:ARG:HA	1:A:209:ARG:HD3	1.76	0.43
1:A:235:ASN:HA	1:A:236:ASN:HA	1.78	0.43
1:A:151:ASP:HB3	1:A:154:PHE:CD2	2.53	0.43
1:A:357:ARG:HH12	1:A:418:GLY:CA	2.31	0.43
1:A:63:LYS:HD2	1:A:64:ASN:HA	2.00	0.43
1:A:315:ARG:HD3	1:A:319:ASP:OD1	2.19	0.42
1:A:332:PRO:HG3	1:A:413:ILE:HG22	2.02	0.42
1:A:403:LEU:HD13	1:A:409:TYR:CZ	2.54	0.42
1:A:514:ARG:HD2	1:A:524:PHE:CE1	2.55	0.42
1:A:514:ARG:HD2	1:A:524:PHE:CZ	2.55	0.42
1:A:61:ASP:CG	4:A:758:HOH:O	2.63	0.42
1:A:489:ARG:NH2	4:A:717:HOH:O	2.18	0.42
1:A:328:PRO:HB3	1:A:420:SER:HB3	2.02	0.42
1:A:335:LEU:HD11	1:A:346:LEU:HD21	2.00	0.42
1:A:43:LEU:HD12	1:A:44:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HD13	1:A:183:LEU:HD21	2.02	0.41
1:A:63:LYS:HA	1:A:64:ASN:HA	1.82	0.41
1:A:360:ILE:H	1:A:360:ILE:HG13	1.54	0.41
1:A:535:VAL:HA	1:A:536:PRO:HD3	1.96	0.41
1:A:152:GLU:OE2	1:A:165:LYS:NZ	2.26	0.41
1:A:389:GLN:HB2	1:A:393:LEU:HD13	2.02	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	509/518 (98%)	486 (96%)	23 (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	446/447 (100%)	417 (94%)	29 (6%)	15	12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	43	LEU
1	A	64	ASN
1	A	65	THR
1	A	67	ILE
1	A	120	GLU
1	A	143	VAL
1	A	206	LEU
1	A	209	ARG
1	A	236	ASN
1	A	270	SER
1	A	317	ASP
1	A	318	ASN
1	A	327	ARG
1	A	339	VAL
1	A	357	ARG
1	A	360	ILE
1	A	366	CYS
1	A	385	HIS
1	A	387	THR
1	A	395	THR
1	A	402	ASP
1	A	416	VAL
1	A	432	VAL
1	A	436	THR
1	A	483	GLN
1	A	489	ARG
1	A	506	LEU
1	A	514	ARG

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	40	GLN
1	A	296	HIS
1	A	385	HIS
1	A	437	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 ⓘ

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	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
2	NAG	B	2	2	14,14,15	0.50	0	17,19,21	0.68	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	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	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(°)
2	B	1	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

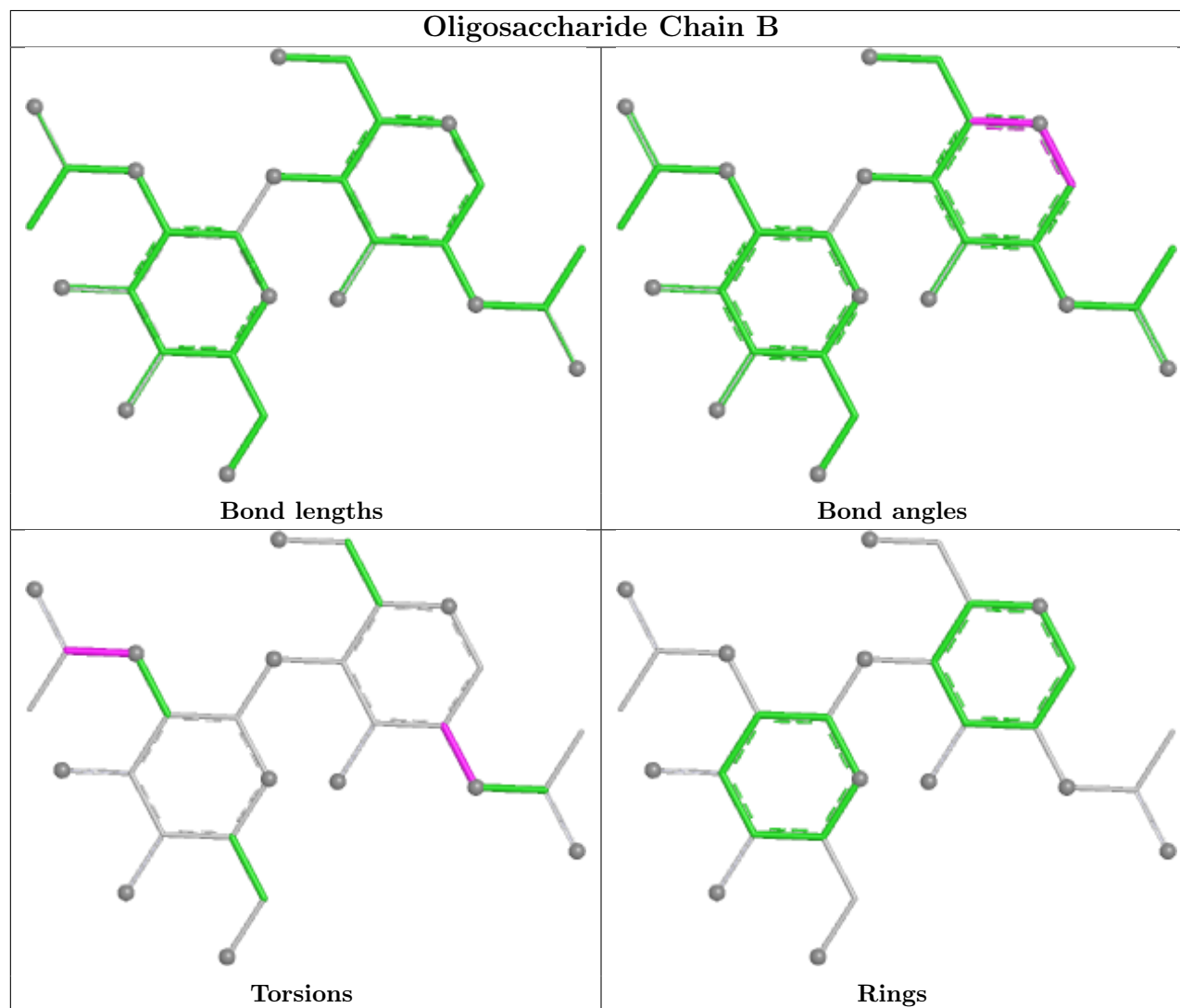
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C1-C2-N2-C7

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	601	1	14,14,15	0.62	0	17,19,21	0.81	0
3	NAG	A	602	1	14,14,15	0.41	0	17,19,21	1.17	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
3	NAG	A	601	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	602	1	-	3/6/23/26	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(°)
3	A	602	NAG	C1-O5-C5	3.31	116.62	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	C8-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O5-C5-C6-O6
3	A	602	NAG	O7-C7-N2-C2
3	A	601	NAG	C3-C2-N2-C7

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/518 (99%)	0.53	77 (15%) 5 6	21, 55, 131, 189	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ASP	4.9
1	A	44	GLY	4.7
1	A	314	PHE	4.6
1	A	374	PRO	4.2
1	A	386	TYR	4.0
1	A	420	SER	4.0
1	A	369	CYS	4.0
1	A	384	VAL	3.9
1	A	419	VAL	3.9
1	A	370	GLY	3.9
1	A	329	PRO	3.8
1	A	43	LEU	3.6
1	A	383	GLY	3.5
1	A	418	GLY	3.4
1	A	155	THR	3.3
1	A	400	ILE	3.2
1	A	382	SER	3.1
1	A	159	ILE	3.1
1	A	422	TYR	3.0
1	A	158	ASP	3.0
1	A	346	LEU	3.0
1	A	325	CYS	3.0
1	A	414	TRP	3.0
1	A	364	VAL	2.9
1	A	321	ALA	2.9
1	A	385	HIS	2.9
1	A	388	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	307	CYS	2.9
1	A	360	ILE	2.9
1	A	421	LYS	2.9
1	A	309	CYS	2.8
1	A	297	SER	2.8
1	A	377	CYS	2.8
1	A	380	CYS	2.8
1	A	153	SER	2.7
1	A	393	LEU	2.7
1	A	366	CYS	2.7
1	A	365	VAL	2.7
1	A	308	THR	2.6
1	A	306	SER	2.6
1	A	279	GLY	2.6
1	A	301	TRP	2.6
1	A	387	THR	2.5
1	A	399	SER	2.5
1	A	348	TRP	2.5
1	A	163	ILE	2.5
1	A	445	ALA	2.5
1	A	413	ILE	2.5
1	A	416	VAL	2.4
1	A	407	THR	2.4
1	A	154	PHE	2.4
1	A	401	THR	2.3
1	A	358	GLN	2.3
1	A	355	GLY	2.3
1	A	342	THR	2.3
1	A	293	CYS	2.3
1	A	316	ALA	2.3
1	A	483	GLN	2.3
1	A	396	THR	2.3
1	A	362	TYR	2.3
1	A	395	THR	2.2
1	A	28	ALA	2.2
1	A	312	GLY	2.2
1	A	65	THR	2.2
1	A	398	VAL	2.2
1	A	356	GLY	2.2
1	A	298	TYR	2.2
1	A	142	PHE	2.1
1	A	40	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	379	PRO	2.1
1	A	406	HIS	2.1
1	A	405	ALA	2.1
1	A	368	LYS	2.1
1	A	391	ASN	2.1
1	A	310	ASP	2.1
1	A	354	THR	2.1
1	A	280	TYR	2.0

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

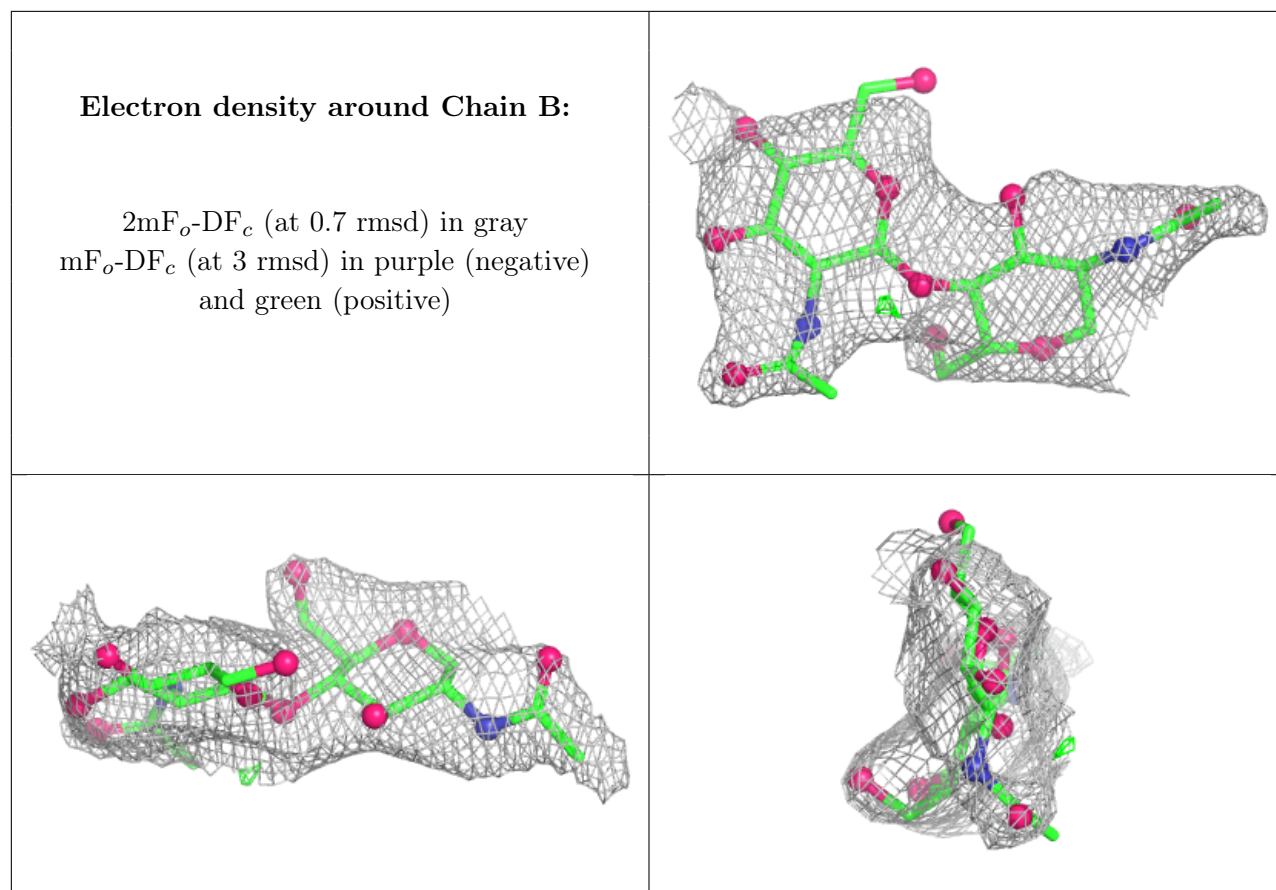
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.70	0.10	97,100,102,102	0
2	NAG	B	1	14/15	0.80	0.10	67,80,88,91	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	602	14/15	0.55	0.14	101,112,119,121	0
3	NAG	A	601	14/15	0.57	0.15	89,103,107,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.