



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6P8I / pdb_00006p8i
Title : N-terminal 5 domains of IGFIIR
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Deposited on : 2019-06-07
Resolution : 2.54 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

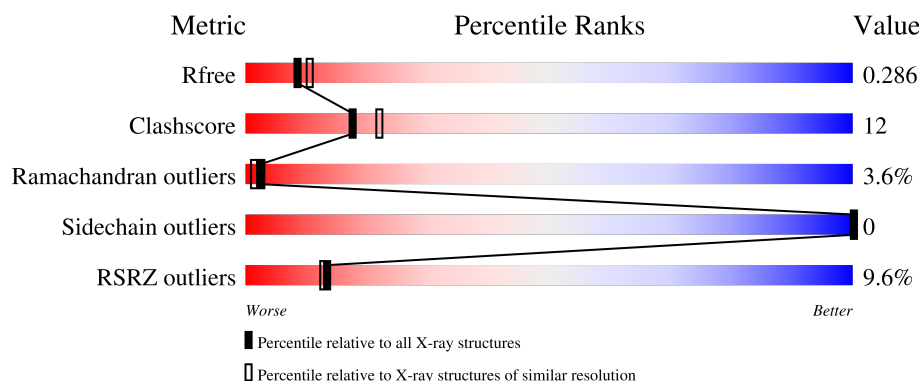
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	735	
2	B	4	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5293 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 Cation-independent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5215	3275	886	1015	39			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P11717
A	0	ALA	-	expression tag	UNP P11717
A	729	ALA	-	expression tag	UNP P11717
A	730	LEU	-	expression tag	UNP P11717
A	731	VAL	-	expression tag	UNP P11717
A	732	PRO	-	expression tag	UNP P11717
A	733	LEU	-	expression tag	UNP P11717

- 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
2	B	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.79Å 66.23Å 123.07Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	39.97 – 2.54 39.97 – 2.54	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.97-2.54) 86.1 (39.97-2.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.54Å)	Xtriage
Refinement program	REFMAC 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.224 , 0.282 0.231 , 0.286	Depositor DCC
R_{free} test set	1971 reflections (7.38%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5293	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: BMA, MAN, 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	0.35	0/5325	0.62	2/7206 (0.0%)

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	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	236	LYS	CD-CE-NZ	-6.77	90.24	111.90
1	A	318	ILE	CA-CB-CG1	-5.78	100.58	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	VAL	Peptide
1	A	435	LYS	Peptide
1	A	459	GLU	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	5215	0	4976	126	2
2	B	50	0	43	1	0
3	A	28	0	0	2	0
All	All	5293	0	5019	127	2

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 12.

All (127) 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:435:LYS:HE2	1:A:437:ASP:CB	1.59	1.32
1:A:435:LYS:CE	1:A:437:ASP:HB3	1.69	1.21
1:A:435:LYS:CE	1:A:437:ASP:CB	2.30	1.06
1:A:435:LYS:HE2	1:A:437:ASP:H	1.26	1.00
1:A:435:LYS:HE2	1:A:437:ASP:N	1.78	0.99
1:A:435:LYS:HE2	1:A:437:ASP:CA	1.96	0.94
1:A:302:VAL:HG21	1:A:434:GLU:OE2	1.66	0.94
1:A:435:LYS:CE	1:A:437:ASP:H	1.82	0.91
1:A:36:SER:HB2	1:A:45:SER:HA	1.59	0.85
1:A:435:LYS:HE2	1:A:437:ASP:HB2	1.55	0.85
1:A:435:LYS:HE3	1:A:437:ASP:HB3	1.61	0.83
1:A:170:THR:HG22	1:A:203:ARG:HG3	1.61	0.82
1:A:454:LEU:HD21	1:A:578:THR:HG21	1.62	0.80
1:A:28:LEU:HB3	1:A:51:HIS:NE2	1.96	0.79
1:A:14:CYS:SG	1:A:34:CYS:HB2	2.22	0.78
1:A:39:ILE:HG22	1:A:41:GLN:H	1.49	0.77
1:A:707:TYR:HE2	1:A:709:GLU:OE1	1.69	0.76
1:A:255:SER:OG	1:A:258:ARG:N	2.19	0.74
1:A:23:THR:HG23	1:A:24:LYS:HD2	1.69	0.72
1:A:71:ARG:HD2	1:A:415:GLY:HA2	1.71	0.71
1:A:302:VAL:CG2	1:A:434:GLU:OE2	2.38	0.71
1:A:435:LYS:O	1:A:436:GLU:CD	2.34	0.69
1:A:28:LEU:HB3	1:A:51:HIS:CD2	2.30	0.66
1:A:51:HIS:HB2	1:A:58:TYR:CD1	2.30	0.66
1:A:362:ARG:HG2	1:A:381:GLY:HA3	1.77	0.66
1:A:723:TYR:HD1	1:A:728:GLU:OE1	1.77	0.66
1:A:109:VAL:O	1:A:369:ARG:NH1	2.30	0.65
1:A:151:LEU:HD22	1:A:154:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:HB2	1:A:531:TYR:HB3	1.78	0.64
1:A:25:ASN:O	1:A:54:LYS:NZ	2.30	0.64
1:A:533:ASP:HB2	1:A:544:LYS:HZ2	1.65	0.62
1:A:303:SER:O	1:A:432:VAL:HG11	2.01	0.60
1:A:435:LYS:NZ	1:A:437:ASP:HB3	2.16	0.60
1:A:256:GLU:O	1:A:698:ARG:NH1	2.36	0.58
1:A:302:VAL:O	3:A:901:HOH:O	2.17	0.58
1:A:435:LYS:CE	1:A:437:ASP:N	2.52	0.57
1:A:517:ILE:HD12	1:A:518:SER:HB2	1.86	0.57
1:A:28:LEU:O	1:A:51:HIS:HD2	1.87	0.57
1:A:304:ILE:HD12	1:A:305:ASP:H	1.70	0.57
1:A:435:LYS:NZ	1:A:437:ASP:O	2.38	0.56
1:A:304:ILE:HD11	1:A:429:TYR:O	2.07	0.55
1:A:435:LYS:CD	1:A:437:ASP:H	2.19	0.55
1:A:28:LEU:HD12	1:A:51:HIS:NE2	2.22	0.55
1:A:302:VAL:HG11	1:A:434:GLU:HB2	1.89	0.54
1:A:281:TYR:OH	1:A:435:LYS:HD3	2.08	0.54
1:A:24:LYS:HE3	1:A:24:LYS:HA	1.89	0.54
1:A:292:THR:OG1	1:A:294:SER:O	2.23	0.53
1:A:725:CYS:O	1:A:727:GLU:N	2.41	0.53
1:A:13:LEU:HD22	1:A:120:TRP:CZ2	2.44	0.53
1:A:40:VAL:HG13	1:A:41:GLN:N	2.24	0.53
2:B:1:NAG:O3	2:B:2:NAG:O5	2.23	0.52
1:A:55:THR:O	1:A:55:THR:OG1	2.27	0.52
1:A:257:ARG:HG3	1:A:699:ASP:HB2	1.90	0.52
1:A:640:ASP:OD1	1:A:640:ASP:N	2.35	0.52
1:A:243:HIS:CG	1:A:270:ASN:HB3	2.46	0.50
1:A:494:ARG:NH1	1:A:496:CYS:HB3	2.26	0.50
1:A:39:ILE:HG22	1:A:41:GLN:N	2.22	0.50
1:A:610:LYS:HB3	1:A:613:GLY:HA2	1.93	0.50
1:A:327:TYR:O	1:A:346:VAL:HA	2.11	0.50
1:A:55:THR:O	1:A:57:THR:N	2.45	0.50
1:A:135:LYS:HG3	1:A:213:PRO:HB2	1.93	0.50
1:A:435:LYS:O	1:A:436:GLU:CG	2.60	0.50
1:A:578:THR:HG22	1:A:580:ALA:H	1.77	0.50
1:A:257:ARG:CG	1:A:699:ASP:HB2	2.41	0.49
1:A:349:VAL:HG22	1:A:357:VAL:HG12	1.93	0.49
1:A:489:GLN:HG3	1:A:492:LYS:HG2	1.94	0.49
1:A:433:LYS:N	1:A:434:GLU:OE1	2.45	0.48
1:A:318:ILE:HA	1:A:326:PHE:O	2.13	0.48
1:A:363:TYR:O	1:A:365:ASN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLN:HB2	1:A:656:LEU:HD11	1.95	0.48
1:A:351:LYS:C	1:A:354:THR:HG21	2.38	0.48
1:A:459:GLU:CB	1:A:461:GLU:HB3	2.43	0.48
1:A:56:ARG:HG2	1:A:58:TYR:CE1	2.49	0.47
1:A:658:LEU:HG	1:A:676:GLY:HA3	1.97	0.47
1:A:432:VAL:CG1	1:A:434:GLU:OE2	2.61	0.47
1:A:290:SER:C	1:A:291:LYS:HD3	2.40	0.47
1:A:515:LYS:HB3	1:A:532:SER:N	2.29	0.47
1:A:555:ASP:OD2	1:A:557:GLU:HG3	2.15	0.47
1:A:54:LYS:O	1:A:55:THR:OG1	2.33	0.47
1:A:457:HIS:O	1:A:457:HIS:ND1	2.45	0.47
1:A:514:GLY:C	1:A:515:LYS:HD2	2.40	0.47
1:A:627:ASN:HB3	1:A:630:GLY:O	2.15	0.47
1:A:320:ASP:OD2	1:A:351:LYS:NZ	2.43	0.47
1:A:432:VAL:HG12	1:A:434:GLU:OE2	2.15	0.47
1:A:88:ASN:HA	1:A:389:PHE:CZ	2.51	0.46
1:A:196:GLY:O	1:A:212:GLN:HG2	2.15	0.46
1:A:101:LYS:HB3	1:A:157:LEU:HD11	1.98	0.46
1:A:147:ARG:N	3:A:902:HOH:O	2.41	0.45
1:A:73:LEU:HD23	1:A:96:ALA:HA	1.97	0.45
1:A:197:THR:HG22	1:A:199:ALA:H	1.81	0.45
1:A:302:VAL:HG11	1:A:434:GLU:CB	2.47	0.45
1:A:343:GLN:O	1:A:362:ARG:HB3	2.17	0.45
1:A:457:HIS:CE1	1:A:727:GLU:OE1	2.71	0.44
1:A:28:LEU:O	1:A:51:HIS:CD2	2.69	0.44
1:A:638:GLN:HA	1:A:639:PRO:HD3	1.87	0.44
1:A:392:MET:HB3	1:A:420:THR:HG23	1.99	0.44
1:A:590:GLU:O	1:A:593:THR:HG22	2.18	0.43
1:A:725:CYS:C	1:A:727:GLU:H	2.26	0.43
1:A:258:ARG:HH12	1:A:276:GLU:CD	2.26	0.43
1:A:304:ILE:HD12	1:A:305:ASP:N	2.32	0.43
1:A:434:GLU:OE1	1:A:434:GLU:N	2.52	0.43
1:A:309:LEU:O	1:A:311:GLN:N	2.52	0.43
1:A:147:ARG:HB3	1:A:284:HIS:HB2	2.01	0.43
1:A:702:VAL:HG12	1:A:723:TYR:HE2	1.83	0.43
1:A:257:ARG:NH2	1:A:697:ASP:OD2	2.48	0.42
1:A:456:ARG:HD3	1:A:462:GLN:O	2.19	0.42
1:A:459:GLU:HB2	1:A:461:GLU:HB3	2.01	0.42
1:A:494:ARG:CZ	1:A:496:CYS:HA	2.49	0.42
1:A:658:LEU:H	1:A:676:GLY:H	1.67	0.42
1:A:245:PRO:HA	1:A:271:CYS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:TYR:O	1:A:325:LEU:HD23	2.18	0.42
1:A:387:SER:OG	1:A:388:GLY:N	2.51	0.42
1:A:606:SER:N	1:A:607:PRO:HD2	2.33	0.42
1:A:610:LYS:CB	1:A:613:GLY:HA2	2.50	0.42
1:A:546:ASN:O	1:A:573:GLU:HA	2.19	0.42
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.84	0.42
1:A:448:ARG:HD3	1:A:584:LEU:HD12	2.02	0.42
1:A:434:GLU:N	1:A:434:GLU:CD	2.78	0.41
1:A:529:LEU:HD21	1:A:531:TYR:CE1	2.55	0.41
1:A:707:TYR:CE2	1:A:709:GLU:OE1	2.60	0.41
1:A:27:VAL:HG13	1:A:51:HIS:O	2.20	0.41
1:A:304:ILE:HD13	1:A:432:VAL:CG2	2.51	0.41
1:A:156:LYS:HE2	1:A:160:ALA:O	2.21	0.41
1:A:94:SER:HB2	1:A:117:TYR:HD1	1.86	0.40
1:A:237:LEU:HD22	1:A:243:HIS:O	2.21	0.40
1:A:127:LYS:N	1:A:127:LYS:HD2	2.36	0.40
1:A:243:HIS:HD2	1:A:711:ASP:OD2	2.05	0.40

All (2) 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:90:ARG:NH2	1:A:318:ILE:CD1[2_655]	1.70	0.50
1:A:597:SER:OG	1:A:640:ASP:OD2[2_444]	2.01	0.19

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	646/735 (88%)	568 (88%)	55 (8%)	23 (4%)	2 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	LYS
1	A	516	PHE
1	A	562	LEU
1	A	614	ALA
1	A	310	ALA
1	A	406	ASP
1	A	524	LYS
1	A	676	GLY
1	A	232	GLU
1	A	342	LYS
1	A	364	HIS
1	A	365	ASN
1	A	436	GLU
1	A	495	GLY
1	A	518	SER
1	A	207	ALA
1	A	381	GLY
1	A	492	LYS
1	A	204	GLY
1	A	238	ASP
1	A	635	SER
1	A	726	PRO
1	A	677	GLY

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	575/629 (91%)	575 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	41	GLN
1	A	89	HIS

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Mol	Chain	Res	Type
1	A	526	ASN
1	A	577	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	B	1	1,2	14,14,15	0.71	1 (7%)	17,19,21	1.10	3 (17%)
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	0.94	0
2	BMA	B	3	2	11,11,12	2.40	6 (54%)	15,15,17	3.23	6 (40%)
2	MAN	B	4	2	11,11,12	0.80	0	15,15,17	1.67	1 (6%)

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	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	1/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C4-C5	5.05	1.63	1.53
2	B	3	BMA	O5-C5	3.36	1.50	1.43
2	B	3	BMA	C1-C2	2.61	1.58	1.52
2	B	3	BMA	C4-C3	2.61	1.59	1.52
2	B	1	NAG	O5-C1	2.47	1.47	1.43
2	B	3	BMA	C2-C3	-2.45	1.48	1.52
2	B	3	BMA	O5-C1	2.09	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-C2-C3	-8.65	97.05	109.64
2	B	3	BMA	C1-O5-C5	-6.15	103.95	112.19
2	B	4	MAN	C1-O5-C5	5.66	119.77	112.19
2	B	3	BMA	O3-C3-C4	3.46	118.52	110.38
2	B	3	BMA	O5-C1-C2	-3.31	102.90	110.79
2	B	3	BMA	O3-C3-C2	2.35	114.84	110.05
2	B	1	NAG	C4-C3-C2	-2.16	107.85	111.02
2	B	1	NAG	C1-O5-C5	2.10	115.00	112.19
2	B	3	BMA	O2-C2-C1	2.10	114.03	109.22
2	B	1	NAG	C1-C2-N2	2.05	113.67	110.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

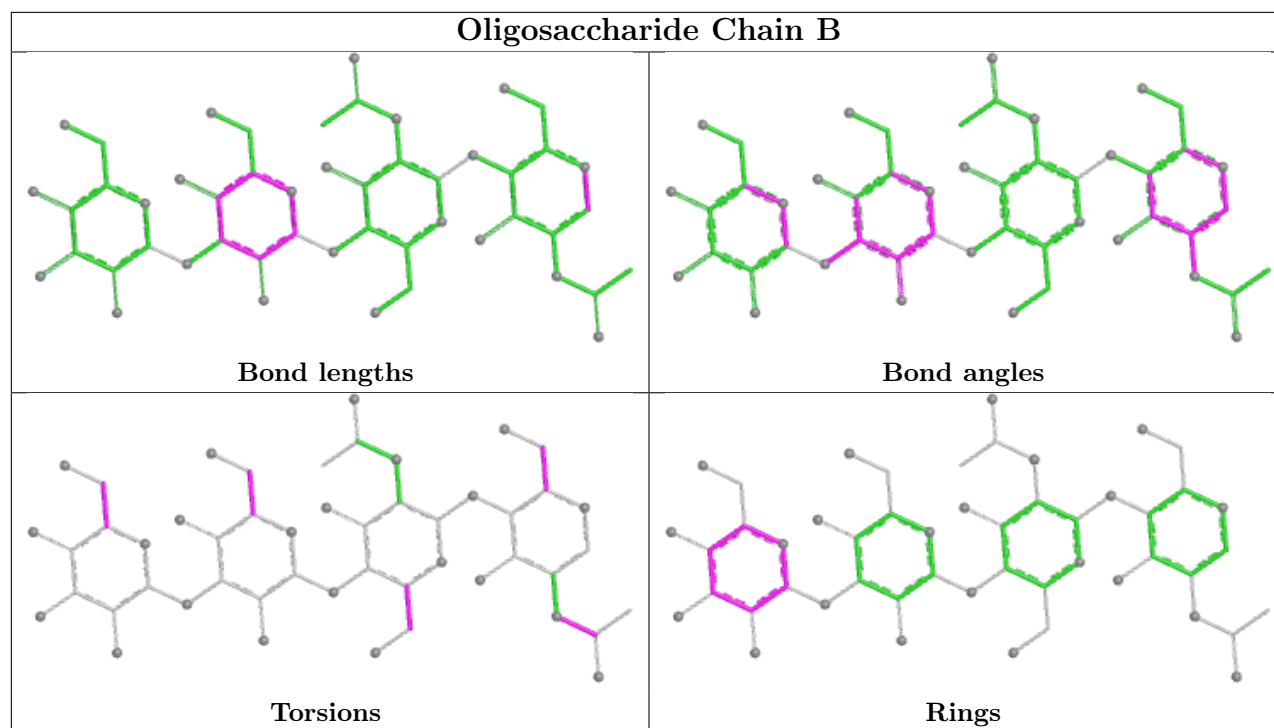
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	1	0

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



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	666/735 (90%)	0.71	64 (9%) 13 13	34, 61, 99, 115	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	ALA	8.5
1	A	729	ALA	5.2
1	A	513	LEU	4.4
1	A	333	GLU	4.1
1	A	332	GLY	3.9
1	A	562	LEU	3.9
1	A	53	LEU	3.9
1	A	496	CYS	3.8
1	A	51	HIS	3.7
1	A	516	PHE	3.7
1	A	728	GLU	3.6
1	A	467	VAL	3.5
1	A	514	GLY	3.4
1	A	517	ILE	3.3
1	A	685	HIS	3.3
1	A	429	TYR	3.3
1	A	88	ASN	3.2
1	A	334	THR	3.0
1	A	364	HIS	3.0
1	A	236	LYS	3.0
1	A	570	CYS	3.0
1	A	650	ASP	2.9
1	A	491	GLY	2.9
1	A	302	VAL	2.8
1	A	363	TYR	2.7
1	A	457	HIS	2.7
1	A	512	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	317	TYR	2.6
1	A	83	ASP	2.5
1	A	335	GLU	2.5
1	A	330	VAL	2.5
1	A	486	ARG	2.5
1	A	331	CYS	2.4
1	A	479	PHE	2.4
1	A	8	ALA	2.4
1	A	310	ALA	2.4
1	A	727	GLU	2.4
1	A	565	SER	2.3
1	A	478	HIS	2.3
1	A	493	ALA	2.3
1	A	322	LYS	2.3
1	A	466	ALA	2.3
1	A	34	CYS	2.3
1	A	329	ASN	2.2
1	A	533	ASP	2.2
1	A	487	VAL	2.2
1	A	379	TYR	2.2
1	A	494	ARG	2.2
1	A	205	HIS	2.1
1	A	234	ALA	2.1
1	A	712	ASN	2.1
1	A	79	THR	2.1
1	A	58	TYR	2.1
1	A	304	ILE	2.1
1	A	384	GLU	2.1
1	A	70	THR	2.1
1	A	676	GLY	2.1
1	A	600	GLY	2.1
1	A	436	GLU	2.0
1	A	80	VAL	2.0
1	A	309	LEU	2.0
1	A	403	ALA	2.0
1	A	354	THR	2.0
1	A	316	SER	2.0

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

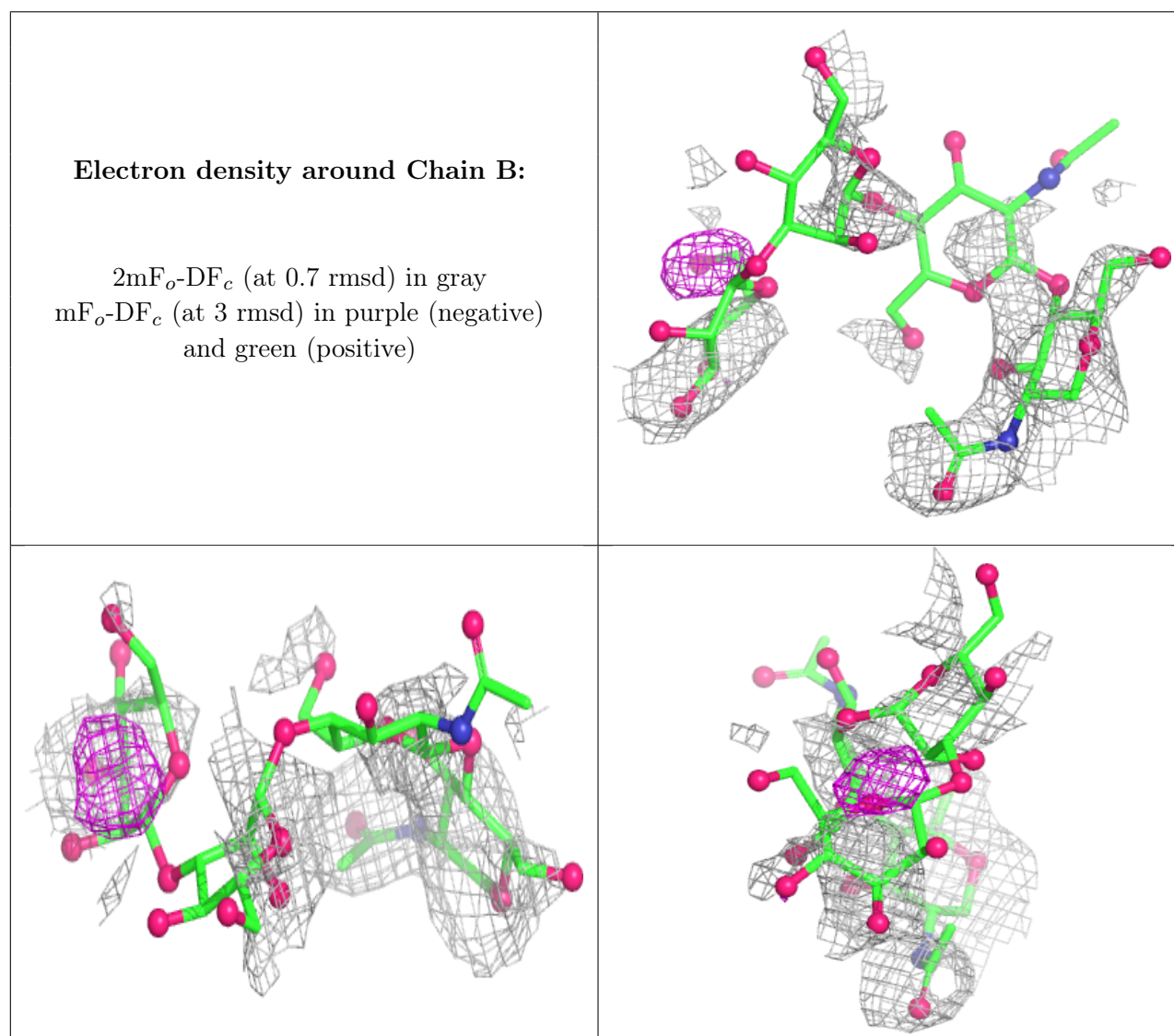
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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	0.44	0.17	146,172,182,188	0
2	BMA	B	3	11/12	0.49	0.19	177,185,196,203	0
2	NAG	B	1	14/15	0.54	0.17	86,115,139,150	0
2	MAN	B	4	11/12	0.78	0.24	111,143,161,164	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.