



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 2X97 / pdb_00002x97
Title : Crystal structure of AnCE-RXP407 complex
Authors : Akif, M.; Georgiadis, D.; Mahajan, A.; Dive, V.; Sturrock, E.D.; Isaac, R.E.; Acharya, K.R.
Deposited on : 2010-03-14
Resolution : 1.85 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

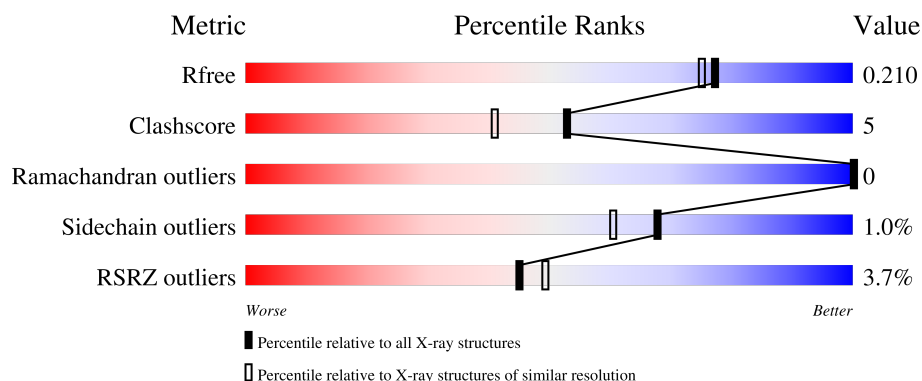
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	598	
2	B	6	

2 Entry composition [i](#)

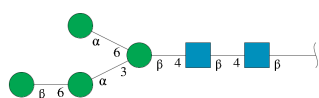
There are 6 unique types of molecules in this entry. The entry contains 5756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANGIOTENSIN CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	598	4883	3124	806	933	20	0	2	0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	6	72	40	2	30	0	0	0

- Molecule 3 is N²-acetyl-N-{(1R)-1-[(S)-[(2S)-3-[(2S)-1-amino-1-oxopropan-2-yl]amino]-2-methyl-3-oxopropyl](hydroxy)phosphoryl]-2-phenylethyl}-L-alpha-asparagine (CCD ID: RX4) (formula: C₂₁H₃₁N₄O₈P).

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

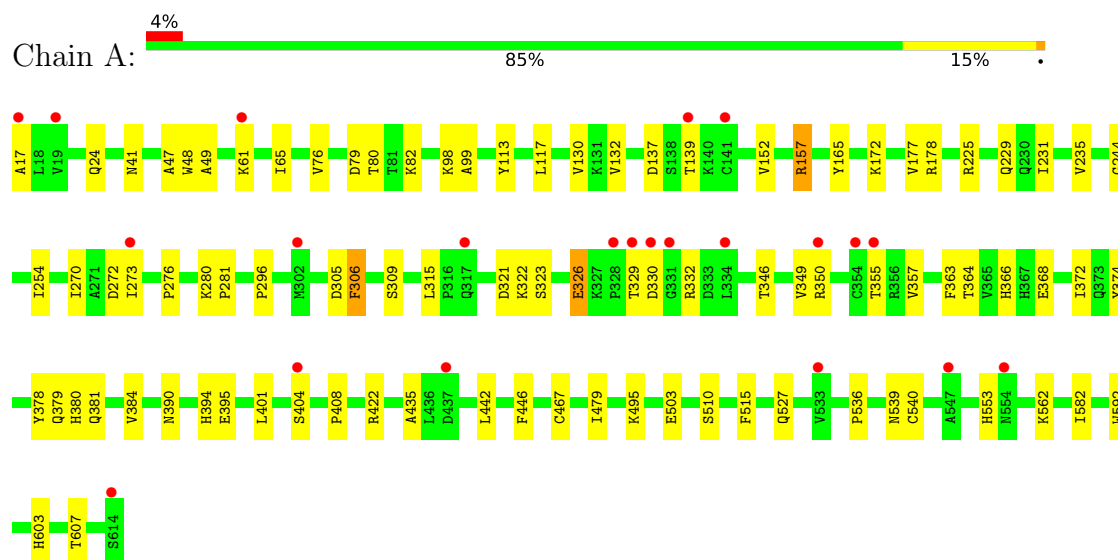
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	738	Total	O	0	0
			738	738		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ANGIOTENSIN CONVERTING ENZYME



• Molecule 2: beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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	H 3	Depositor
Cell constants a, b, c, α , β , γ	173.09Å 173.09Å 101.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.62 – 1.85 31.62 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.3 (31.62-1.85) 73.8 (31.62-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.172 , 0.201 0.182 , 0.210	Depositor DCC
R_{free} test set	3564 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.018 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.011 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.014 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.028 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.026 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.116 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5756	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MAN, BMA, NAG, RX4, ZN

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	1.57	31/5015 (0.6%)	1.21	14/6796 (0.2%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLN	CB-CG	-8.87	1.25	1.52
1	A	346	THR	CB-OG1	7.87	1.56	1.43
1	A	157	ARG	CZ-NH1	7.34	1.43	1.32
1	A	562	LYS	C-O	6.88	1.30	1.24
1	A	527	GLN	CD-OE1	6.87	1.36	1.23
1	A	379	GLN	CD-OE1	6.52	1.35	1.23
1	A	553	HIS	ND1-CE1	6.47	1.39	1.32
1	A	582	ILE	CA-CB	6.12	1.62	1.54
1	A	366	HIS	ND1-CE1	6.08	1.38	1.32
1	A	607	THR	CB-OG1	6.08	1.53	1.43
1	A	254	ILE	CA-C	5.75	1.58	1.53
1	A	380	HIS	ND1-CE1	5.75	1.38	1.32
1	A	381	GLN	CD-OE1	5.73	1.34	1.23
1	A	130	VAL	CA-CB	5.60	1.60	1.54
1	A	384	VAL	N-CA	5.55	1.53	1.46
1	A	99	ALA	N-CA	5.54	1.53	1.46
1	A	231	ILE	CA-CB	5.53	1.61	1.54
1	A	49	ALA	CA-CB	5.52	1.61	1.53
1	A	346	THR	CA-C	5.50	1.59	1.52
1	A	357	VAL	CA-CB	5.49	1.60	1.53
1	A	244	GLY	N-CA	5.49	1.50	1.45
1	A	442	LEU	CA-C	5.45	1.59	1.52
1	A	323	SER	N-CA	5.44	1.52	1.46
1	A	41	ASN	CG-OD1	5.21	1.33	1.23
1	A	306	PHE	CA-CB	5.17	1.61	1.53
1	A	390	ASN	CA-C	5.07	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	CYS	CB-SG	5.06	1.98	1.81
1	A	435	ALA	CA-CB	5.06	1.61	1.53
1	A	235	VAL	CA-C	5.05	1.59	1.52
1	A	326	GLU	CA-C	-5.03	1.46	1.52
1	A	363	PHE	C-O	-5.03	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	HIS	CB-CG-CD2	-7.04	122.05	131.20
1	A	177	VAL	N-CA-CB	-6.92	103.15	112.22
1	A	157	ARG	NE-CZ-NH2	-6.92	112.98	119.20
1	A	603	HIS	CB-CG-CD2	-6.08	123.29	131.20
1	A	366	HIS	CB-CG-CD2	-6.04	123.34	131.20
1	A	380	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	A	553	HIS	CB-CG-ND1	5.92	131.58	122.70
1	A	177	VAL	CG1-CB-CG2	5.74	123.42	110.80
1	A	374	TYR	N-CA-C	-5.61	105.25	111.36
1	A	390	ASN	CB-CA-C	5.59	118.63	109.97
1	A	515	PHE	N-CA-C	5.33	117.17	111.36
1	A	380	HIS	CB-CG-ND1	5.24	130.56	122.70
1	A	603	HIS	CB-CG-ND1	5.19	130.48	122.70
1	A	47	ALA	N-CA-C	-5.08	105.82	111.36

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	4883	0	4677	49	0
2	B	72	0	61	0	0
3	A	34	0	29	1	0
4	A	1	0	0	0	0
5	A	28	0	26	0	0
6	A	738	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5756	0	4793	49	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 5.

All (49) 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:322:LYS:HB2	1:A:350:ARG:HD3	1.34	1.08
1:A:322:LYS:CB	1:A:350:ARG:HD3	1.86	1.06
1:A:270:ILE:HB	1:A:273:ILE:HD11	1.40	1.01
1:A:178:ARG:NH1	6:A:2267:HOH:O	2.03	0.87
1:A:322:LYS:HB3	1:A:350:ARG:HD3	1.67	0.77
1:A:61:LYS:O	1:A:65:ILE:HG12	1.89	0.72
1:A:270:ILE:HB	1:A:273:ILE:CD1	2.19	0.70
1:A:296:PRO:HA	1:A:355:THR:HG21	1.77	0.65
1:A:305:ASP:OD1	6:A:2448:HOH:O	2.13	0.65
1:A:270:ILE:CB	1:A:273:ILE:HD11	2.21	0.62
1:A:270:ILE:O	1:A:273:ILE:HG12	1.99	0.61
1:A:270:ILE:O	1:A:273:ILE:CG1	2.48	0.61
1:A:98:LYS:NZ	6:A:2164:HOH:O	2.35	0.60
1:A:306:PHE:CD2	1:A:401:LEU:HD13	2.37	0.59
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.40	0.57
1:A:157:ARG:NH2	1:A:272:ASP:OD1	2.38	0.57
1:A:79:ASP:HA	1:A:82:LYS:HD3	1.87	0.57
1:A:321:ASP:OD1	6:A:2461:HOH:O	2.18	0.57
1:A:296:PRO:HG2	1:A:326:GLU:HG2	1.89	0.55
1:A:330:ASP:OD1	1:A:332:ARG:HD3	2.08	0.54
1:A:422:ARG:NH2	6:A:2550:HOH:O	2.31	0.53
1:A:17:ALA:HB3	6:A:2002:HOH:O	2.10	0.52
1:A:270:ILE:O	1:A:273:ILE:HG13	2.12	0.49
1:A:137:ASP:C	1:A:139:THR:H	2.21	0.48
1:A:296:PRO:HG3	1:A:355:THR:HG22	1.96	0.48
1:A:296:PRO:CA	1:A:355:THR:HG21	2.44	0.47
1:A:395:GLU:HB2	1:A:510:SER:HB2	1.97	0.47
1:A:422:ARG:O	1:A:422:ARG:HG2	2.15	0.47
1:A:137:ASP:OD1	1:A:139:THR:HB	2.15	0.47
1:A:280:LYS:HB3	1:A:281:PRO:HD2	1.97	0.46
1:A:422:ARG:NH2	1:A:536:PRO:HG3	2.30	0.46
1:A:306:PHE:HZ	1:A:404:SER:HG	1.59	0.46
1:A:306:PHE:CZ	1:A:404:SER:OG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:O	1:A:80:THR:HG23	2.16	0.45
1:A:132:VAL:HG12	1:A:172:LYS:HE3	1.98	0.45
1:A:296:PRO:HG3	1:A:355:THR:CG2	2.47	0.44
1:A:225:ARG:O	1:A:229:GLN:HG2	2.18	0.44
1:A:408:PRO:HD2	1:A:539:ASN:OD1	2.18	0.44
1:A:495:LYS:NZ	3:A:1615:RX4:HAD2	2.15	0.43
1:A:329:THR:HB	6:A:2473:HOH:O	2.18	0.43
1:A:364:THR:O	1:A:368:GLU:HG2	2.18	0.43
1:A:305:ASP:O	1:A:309:SER:HB3	2.19	0.43
1:A:479:ILE:C	1:A:479:ILE:HD12	2.45	0.42
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.54	0.42
1:A:270:ILE:HB	1:A:273:ILE:CG1	2.49	0.42
1:A:315:LEU:CD2	1:A:372:ILE:HG21	2.49	0.42
1:A:349:VAL:C	1:A:350:ARG:HG3	2.45	0.41
1:A:48:TRP:CD1	1:A:48:TRP:C	2.99	0.40
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.56	0.40

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	598/598 (100%)	586 (98%)	12 (2%)	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	521/520 (100%)	516 (99%)	5 (1%)	68	60

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

Mol	Chain	Res	Type
1	A	378	TYR
1	A	394	HIS
1	A	446	PHE
1	A	503	GLU
1	A	540	CYS

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	159	HIS
1	A	229	GLN
1	A	377	GLN
1	A	430	GLN

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 ⓘ

6 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	0.92	1 (7%)	17,19,21	1.43	3 (17%)
2	NAG	B	2	2	14,14,15	0.80	0	17,19,21	2.02	5 (29%)
2	BMA	B	3	2	11,11,12	0.55	0	15,15,17	1.11	1 (6%)
2	MAN	B	4	2	11,11,12	0.79	0	15,15,17	1.13	1 (6%)
2	BMA	B	5	2	11,11,12	0.90	0	15,15,17	2.58	6 (40%)
2	MAN	B	6	2	11,11,12	1.49	2 (18%)	15,15,17	2.50	8 (53%)

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	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	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	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	1/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	MAN	C2-C3	3.42	1.57	1.52
2	B	6	MAN	C1-C2	2.60	1.58	1.52
2	B	1	NAG	C1-C2	2.03	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	BMA	O3-C3-C4	5.07	122.34	110.38
2	B	6	MAN	C1-C2-C3	4.68	116.46	109.64
2	B	5	BMA	O2-C2-C3	-4.46	100.92	110.15
2	B	5	BMA	C2-C3-C4	-4.25	103.38	110.86
2	B	2	NAG	O6-C6-C5	-3.93	97.96	111.33
2	B	6	MAN	O5-C5-C6	3.83	115.11	107.66
2	B	6	MAN	C1-O5-C5	-3.74	107.17	112.19
2	B	2	NAG	C1-O5-C5	3.65	117.08	112.19
2	B	5	BMA	C3-C4-C5	-3.64	103.64	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	MAN	O3-C3-C2	3.41	117.02	110.05
2	B	2	NAG	C6-C5-C4	-3.35	104.79	113.02
2	B	2	NAG	O4-C4-C5	-3.12	101.63	109.32
2	B	1	NAG	C1-O5-C5	3.11	116.35	112.19
2	B	3	BMA	O5-C5-C6	3.04	113.58	107.66
2	B	5	BMA	C1-C2-C3	2.88	113.84	109.64
2	B	1	NAG	O5-C1-C2	-2.81	106.95	111.29
2	B	2	NAG	C2-N2-C7	2.80	126.66	122.90
2	B	6	MAN	O4-C4-C5	2.75	116.09	109.32
2	B	6	MAN	O4-C4-C3	-2.53	104.41	110.38
2	B	4	MAN	C1-O5-C5	2.33	115.31	112.19
2	B	6	MAN	O2-C2-C1	2.31	114.51	109.22
2	B	6	MAN	C6-C5-C4	2.18	118.37	113.02
2	B	5	BMA	O4-C4-C5	2.06	114.40	109.32
2	B	1	NAG	O6-C6-C5	-2.00	104.51	111.33

There are no chirality outliers.

All (11) torsion outliers are listed below:

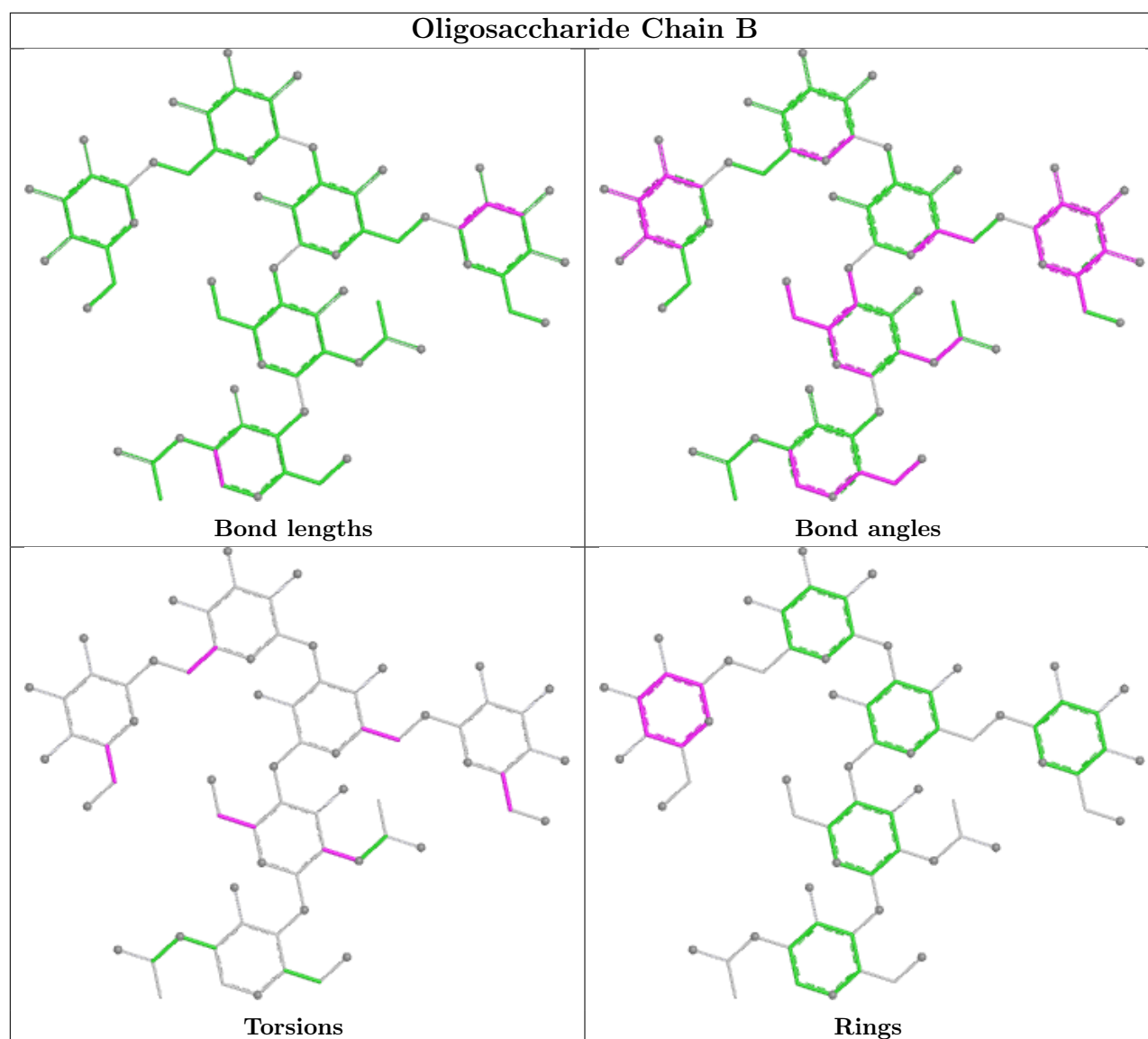
Mol	Chain	Res	Type	Atoms
2	B	6	MAN	O5-C5-C6-O6
2	B	5	BMA	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	5	BMA	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	B	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
3	RX4	A	1615	4	31,34,34	1.52	7 (22%)	38,47,47	1.75	10 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1623	1	14,14,15	0.57	0	17,19,21	0.64	0
5	NAG	A	1622	1	14,14,15	0.64	0	17,19,21	1.68	3 (17%)

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	RX4	A	1615	4	-	5/38/43/43	0/1/1/1
5	NAG	A	1623	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1622	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1615	RX4	CA-N	2.91	1.51	1.45
3	A	1615	RX4	CAA-CAX	2.69	1.56	1.50
3	A	1615	RX4	CAB-CBD	2.54	1.61	1.52
3	A	1615	RX4	CAS-CBG	2.48	1.58	1.54
3	A	1615	RX4	CBF-NAU	2.45	1.51	1.45
3	A	1615	RX4	O-C	2.43	1.28	1.23
3	A	1615	RX4	CBD-CBA	2.43	1.58	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1615	RX4	CAM-CAN-CAP	-4.78	114.34	120.24
3	A	1615	RX4	CBC-CAS-CBG	-3.51	105.69	113.34
5	A	1622	NAG	C1-C2-N2	-3.33	105.19	110.43
5	A	1622	NAG	C1-O5-C5	3.26	116.55	112.19
5	A	1622	NAG	C4-C3-C2	-3.26	106.25	111.02
3	A	1615	RX4	CAB-CBD-CBA	-3.22	103.71	109.64
3	A	1615	RX4	CAO-CAM-CAN	2.81	123.72	119.87
3	A	1615	RX4	CAS-CBC-CAP	-2.67	115.94	120.90
3	A	1615	RX4	CBB-CBF-NAU	-2.53	104.26	111.11
3	A	1615	RX4	CAO-CAQ-CBC	-2.47	117.13	120.61
3	A	1615	RX4	CBF-CAR-CAZ	-2.36	106.12	112.75
3	A	1615	RX4	OAG-CAZ-CAR	-2.29	115.81	122.84
3	A	1615	RX4	CAQ-CBC-CAP	2.10	121.36	118.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

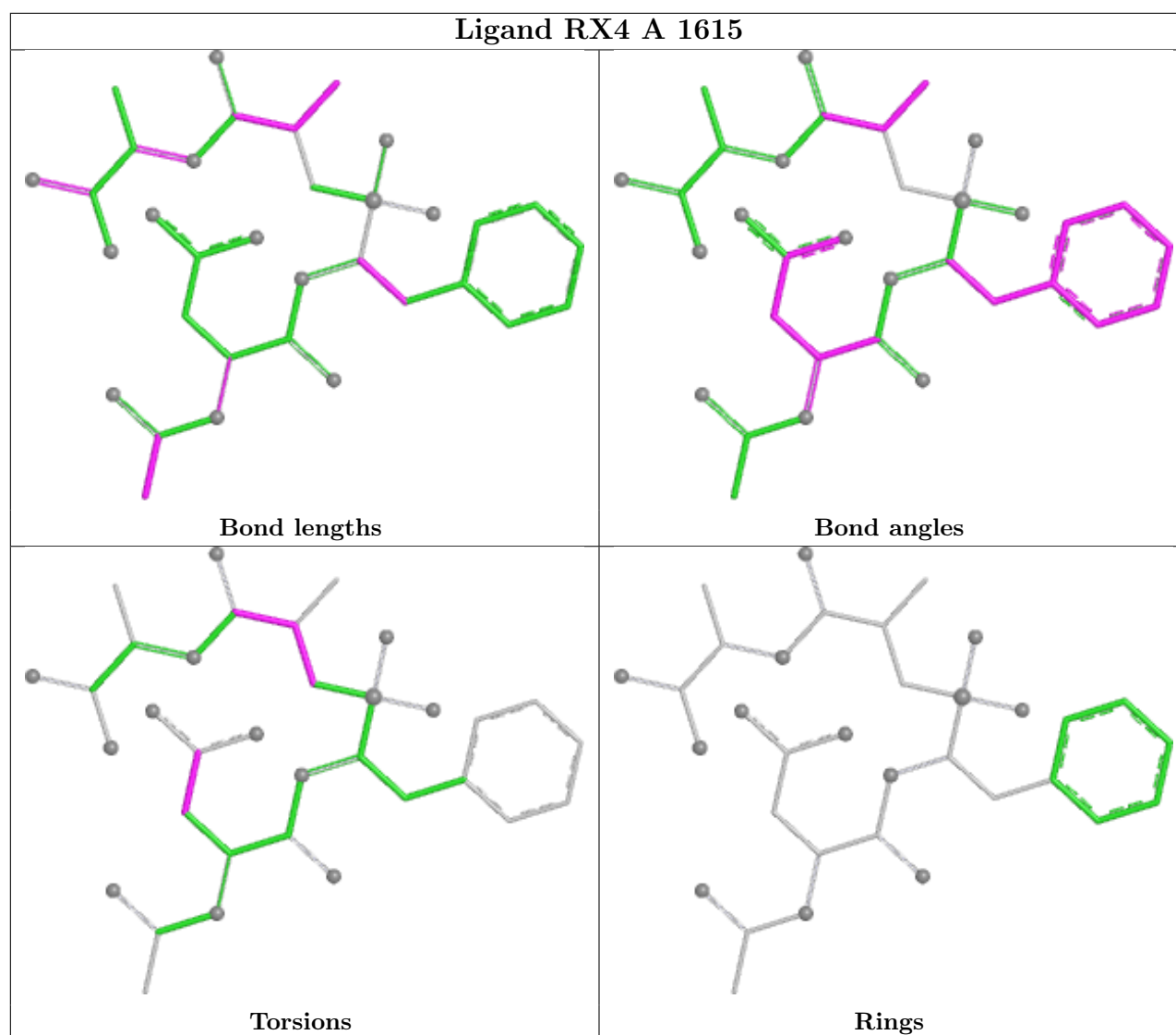
Mol	Chain	Res	Type	Atoms
5	A	1623	NAG	O5-C5-C6-O6
5	A	1623	NAG	C4-C5-C6-O6
3	A	1615	RX4	CBF-CAR-CAZ-OAG
3	A	1615	RX4	OAH-CBA-CBD-CAT
3	A	1615	RX4	N-CBA-CBD-CAT
3	A	1615	RX4	CBF-CAR-CAZ-OAK
3	A	1615	RX4	P1-CAT-CBD-CBA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1615	RX4	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	598/598 (100%)	0.10	22 (3%) 45 49	16, 25, 40, 52	9 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	THR	7.8
1	A	331	GLY	7.1
1	A	354	CYS	5.7
1	A	273	ILE	4.4
1	A	404	SER	4.2
1	A	334	LEU	3.7
1	A	355	THR	3.4
1	A	547	ALA	3.3
1	A	139	THR	3.3
1	A	437	ASP	3.2
1	A	533	VAL	3.0
1	A	317	GLN	2.9
1	A	350	ARG	2.8
1	A	330	ASP	2.8
1	A	328	PRO	2.6
1	A	141	CYS	2.5
1	A	614	SER	2.5
1	A	19	VAL	2.4
1	A	302	MET	2.4
1	A	17	ALA	2.3
1	A	61	LYS	2.1
1	A	554	ASN	2.0

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

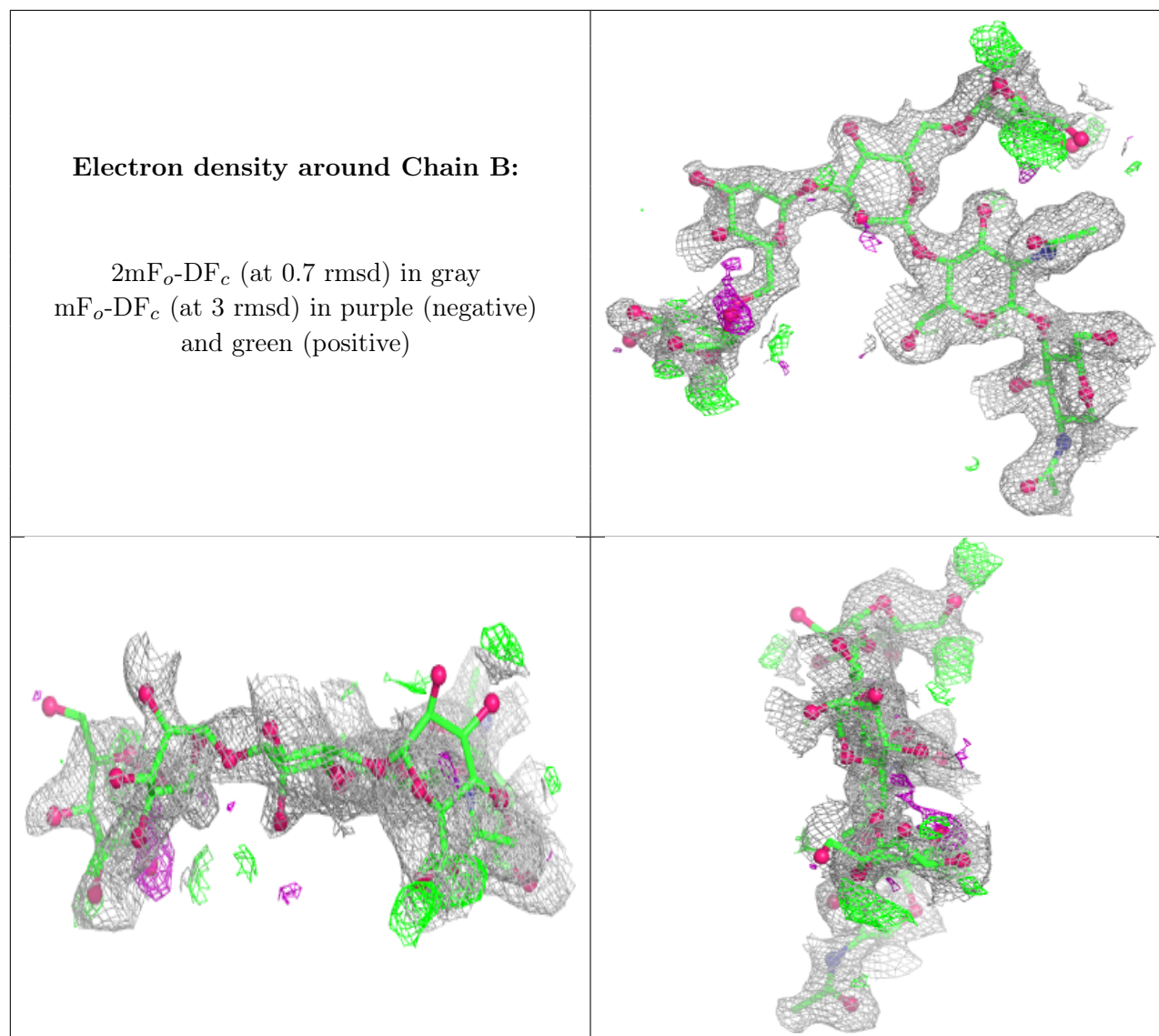
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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	MAN	B	6	11/12	0.69	0.24	64,68,70,71	0
2	BMA	B	5	11/12	0.75	0.21	52,57,66,68	0
2	MAN	B	4	11/12	0.93	0.13	43,45,49,51	0
2	BMA	B	3	11/12	0.94	0.11	38,43,53,58	0
2	NAG	B	2	14/15	0.96	0.07	24,29,37,40	0
2	NAG	B	1	14/15	0.97	0.07	22,26,29,30	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.



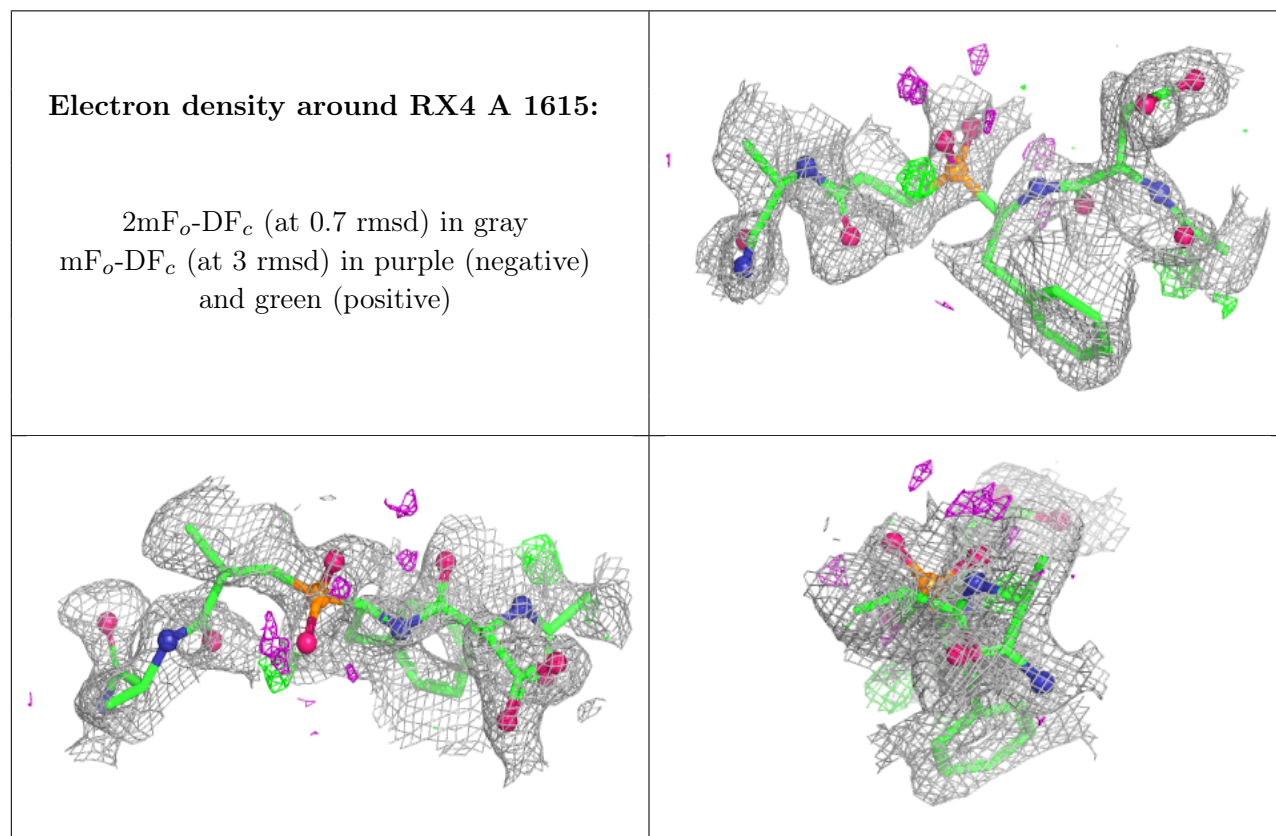
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
5	NAG	A	1622	14/15	0.76	0.29	39,42,46,46	14
5	NAG	A	1623	14/15	0.84	0.18	44,45,45,45	14
3	RX4	A	1615	34/34	0.96	0.09	17,23,36,38	0
4	ZN	A	1616	1/1	0.99	0.02	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.