



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:54 PM UTC

PDB ID : 7AKK / pdb_00007akk
Title : Structure of a complement factor-receptor complex
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Deposited on : 2020-10-01
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

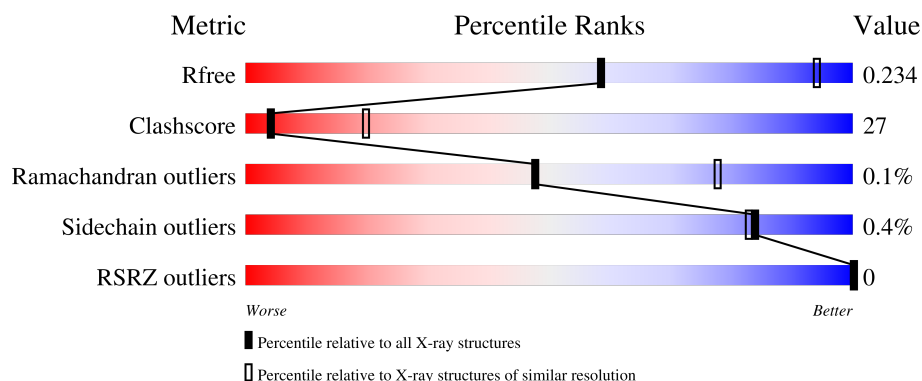
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



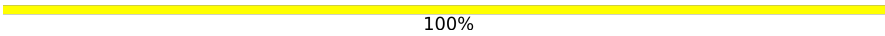
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	B	645	
1	C	645	
2	A	898	
2	E	898	
3	D	195	

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Mol	Chain	Length	Quality of chain
3	H	195	 56% 38% 5%
4	I	3	 100%
5	J	4	 50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24012 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	645	Total	C	N	O	S	0	0	0
			5024	3198	851	960	15			
1	C	645	Total	C	N	O	S	0	0	0
			5024	3198	851	960	15			

- Molecule 2 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	842	Total	C	N	O	S	0	0	0
			6736	4276	1128	1295	37			
2	E	504	Total	C	N	O	S	0	0	0
			4084	2585	684	789	26			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	LYS	deletion	UNP P01024
A	?	-	ILE	deletion	UNP P01024
A	?	-	THR	deletion	UNP P01024
A	?	-	HIS	deletion	UNP P01024
A	?	-	ARG	deletion	UNP P01024
A	?	-	ILE	deletion	UNP P01024
A	?	-	HIS	deletion	UNP P01024
A	?	-	TRP	deletion	UNP P01024
A	?	-	GLU	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	ALA	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	LEU	deletion	UNP P01024

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P01024
E	?	-	ARG	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	LYS	deletion	UNP P01024
E	?	-	ILE	deletion	UNP P01024
E	?	-	THR	deletion	UNP P01024
E	?	-	HIS	deletion	UNP P01024
E	?	-	ARG	deletion	UNP P01024
E	?	-	ILE	deletion	UNP P01024
E	?	-	HIS	deletion	UNP P01024
E	?	-	TRP	deletion	UNP P01024
E	?	-	GLU	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	ALA	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	LEU	deletion	UNP P01024
E	?	-	LEU	deletion	UNP P01024

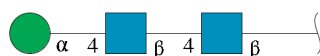
- Molecule 3 is a protein called Integrin alpha-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	185	Total	C	N	O	S	0	0	0
			1499	951	267	278	3			
3	H	185	Total	C	N	O	S	0	0	0
			1499	951	267	278	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	128	SER	CYS	engineered mutation	UNP P11215
D	316	GLY	ILE	engineered mutation	UNP P11215
H	128	SER	CYS	engineered mutation	UNP P11215
H	316	GLY	ILE	engineered mutation	UNP P11215

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



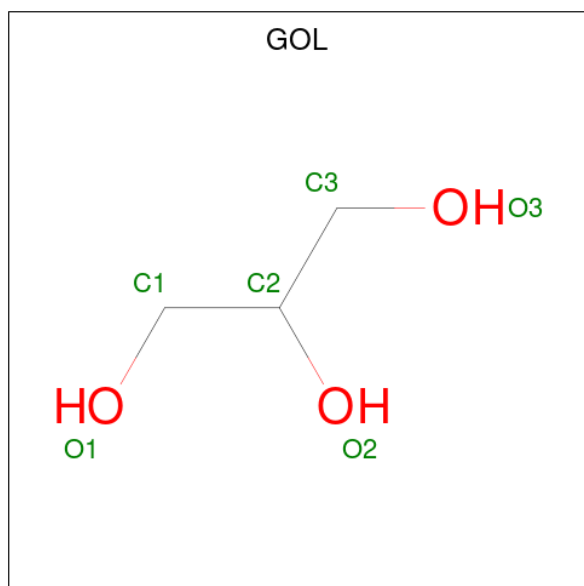
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-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
5	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

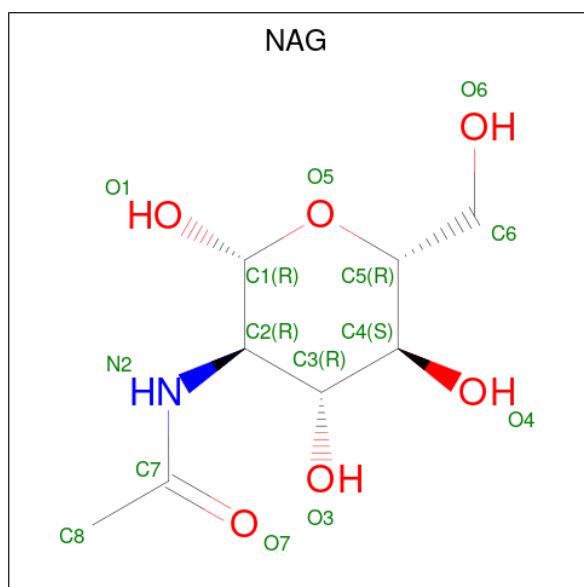
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0
7	C	1	Total K 1 1	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	6	Total O 6 6	0	0
10	A	7	Total O 7 7	0	0

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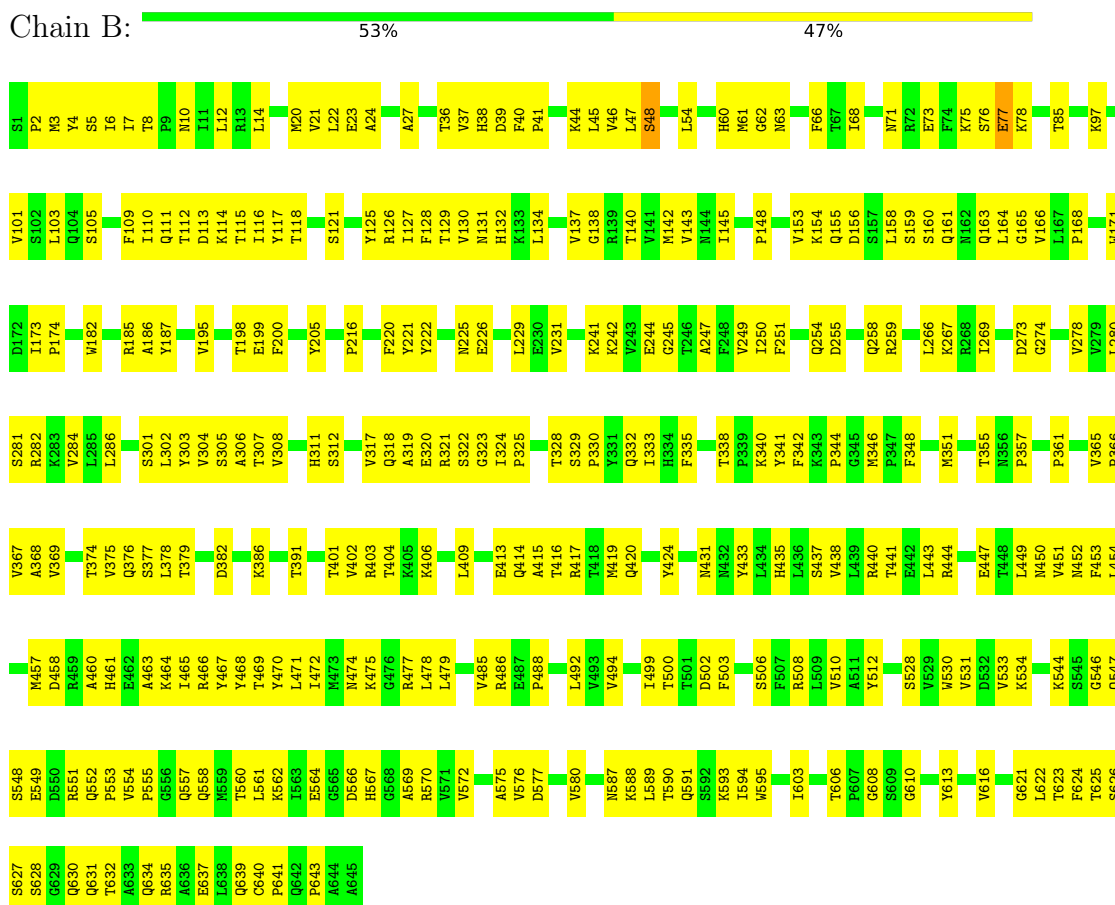
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	O	0	0
			2	2		
10	C	4	Total	O	0	0
			4	4		
10	E	2	Total	O	0	0
			2	2		

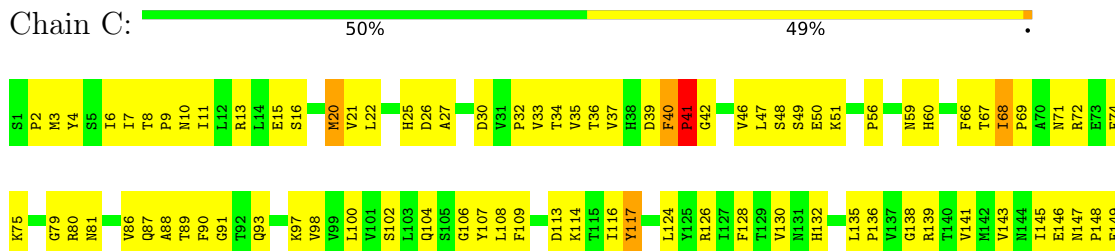
3 Residue-property plots

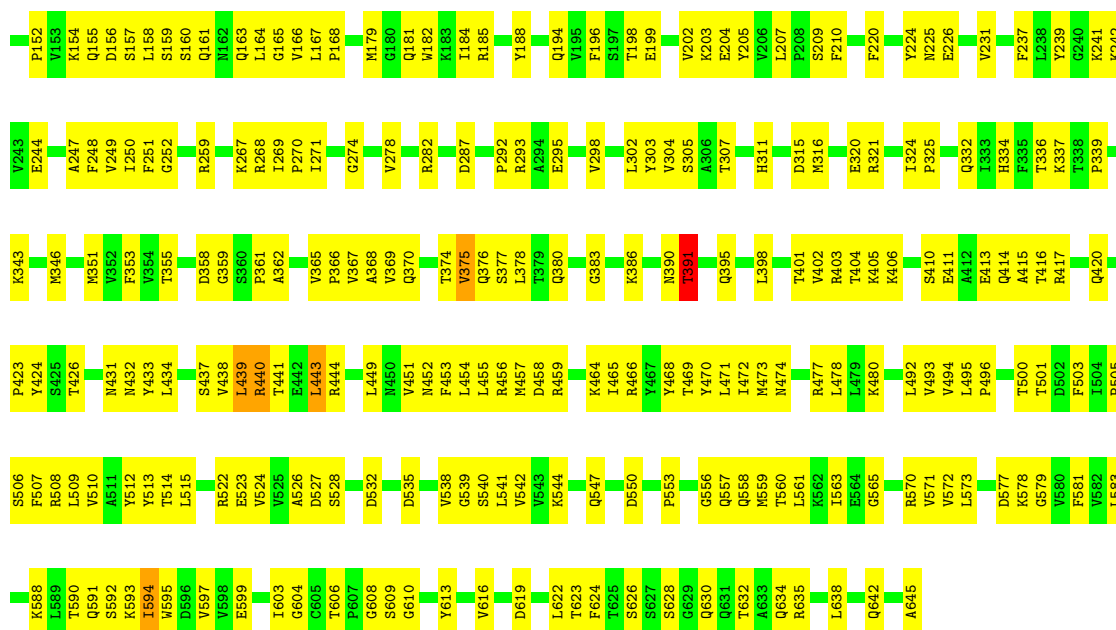
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Complement C3 beta chain



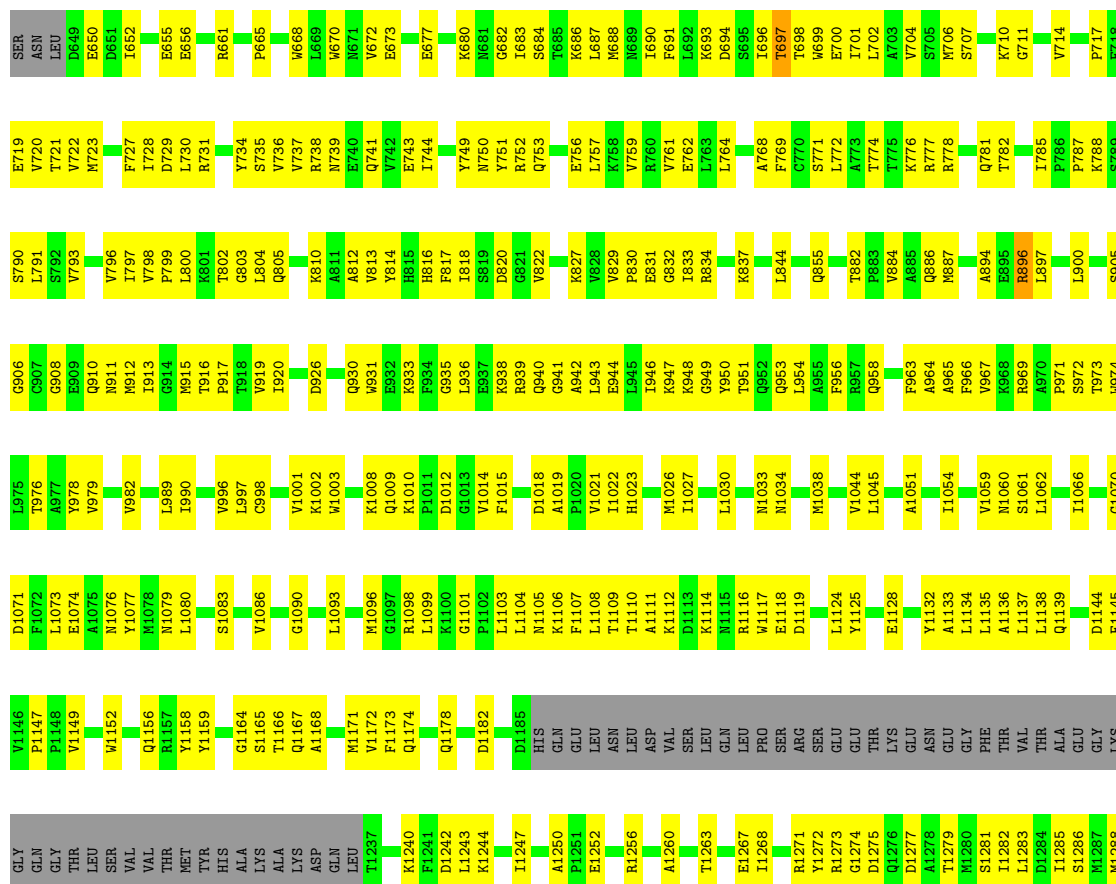
- Molecule 1: Complement C3 beta chain

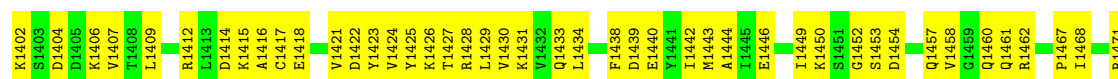




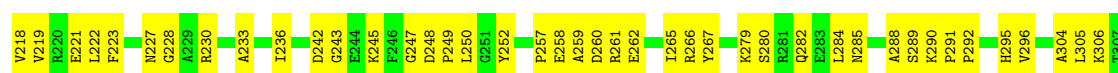
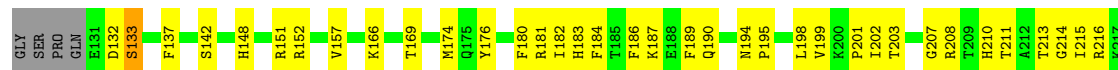
• Molecule 2: Complement C3b alpha' chain

Chain A: 47% 46% 6%





• Molecule 3: Integrin alpha-M



• Molecule 3: Integrin alpha-M



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



• Molecule 5: beta-D-mannopyranose-(1-6)-alpha-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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.29Å 150.73Å 111.30Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	53.77 – 3.40 53.77 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (53.77-3.40) 99.3 (53.77-3.40)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.192 , 0.229 0.192 , 0.234	Depositor DCC
R_{free} test set	2520 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	105.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.109 for l,k,-h 0.117 for h,-k,-l 0.326 for l,-k,h	Xtriage
Reported twinning fraction	0.500 for l,-k,h	Depositor
Outliers	0 of 50383 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24012	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG, GOL, MAN, BMA, K

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	B	0.60	0/5126	0.86	2/6966 (0.0%)
1	C	0.59	1/5126 (0.0%)	0.87	5/6966 (0.1%)
2	A	0.51	0/6871	0.77	4/9303 (0.0%)
2	E	0.56	0/4164	0.79	0/5629
3	D	0.50	0/1527	0.77	1/2054 (0.0%)
3	H	0.60	0/1527	0.86	0/2054
All	All	0.56	1/24341 (0.0%)	0.82	12/32972 (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	B	0	1
1	C	0	1
2	A	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	TYR	C-N	5.80	1.45	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	697	THR	CA-CB-OG1	-8.72	96.52	109.60
1	C	41	PRO	CA-N-CD	-7.24	101.87	112.00
3	D	133	SER	N-CA-C	6.58	118.78	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	MET	CB-CG-SD	-5.78	95.36	112.70
1	C	391	THR	CA-C-N	-5.35	112.89	120.49

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	817	PHE	Peptide
1	B	640	CYS	Peptide
1	C	40	PHE	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	B	5024	0	5084	287	0
1	C	5024	0	5084	339	1
2	A	6736	0	6668	374	2
2	E	4084	0	4022	257	0
3	D	1499	0	1509	67	1
3	H	1499	0	1511	73	2
4	I	39	0	33	2	0
5	J	50	0	43	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	E	6	0	8	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	D	1	0	0	0	0
8	H	1	0	0	0	0
9	E	14	0	13	0	0
10	A	7	0	0	0	0
10	B	6	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
10	E	2	0	0	0	0
All	All	24012	0	23991	1313	3

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 27.

The worst 5 of 1313 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLN:HG3	1:C:401:THR:HB	1.14	1.12
1:C:369:VAL:H	1:C:375:VAL:CG2	1.65	1.09
1:C:369:VAL:H	1:C:375:VAL:HG21	0.94	1.07
1:C:369:VAL:HG22	1:C:375:VAL:HG11	1.34	1.07
1:B:155:GLN:HE21	2:E:804:LEU:HD13	1.13	1.06

All (3) 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)
2:A:756:GLU:OE2	3:H:300:ASN:ND2[2_747]	1.93	0.27
2:A:1428:ARG:NH2	3:H:191:ASN:O[1_455]	2.07	0.13
3:D:249:PRO:O	1:C:71:ASN:ND2[2_657]	2.08	0.12

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	B	643/645 (100%)	609 (95%)	34 (5%)	0	100	100
1	C	643/645 (100%)	617 (96%)	25 (4%)	1 (0%)	43	71
2	A	836/898 (93%)	743 (89%)	92 (11%)	1 (0%)	48	78
2	E	498/898 (56%)	441 (89%)	57 (11%)	0	100	100
3	D	183/195 (94%)	169 (92%)	14 (8%)	0	100	100
3	H	183/195 (94%)	173 (94%)	9 (5%)	1 (0%)	24	54
All	All	2986/3476 (86%)	2752 (92%)	231 (8%)	3 (0%)	48	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	PRO
2	A	656	GLU
3	H	177	SER

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	B	567/567 (100%)	565 (100%)	2 (0%)	84	83
1	C	567/567 (100%)	559 (99%)	8 (1%)	59	70
2	A	745/794 (94%)	745 (100%)	0	100	100
2	E	463/794 (58%)	463 (100%)	0	100	100
3	D	166/172 (96%)	166 (100%)	0	100	100
3	H	166/172 (96%)	166 (100%)	0	100	100
All	All	2674/3066 (87%)	2664 (100%)	10 (0%)	84	83

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	440	ARG
1	C	443	LEU
1	C	594	ILE
1	C	374	THR
1	C	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	ASN
1	C	420	GLN
3	H	175	GLN
1	C	155	GLN

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Mol	Chain	Res	Type
1	C	193	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 ⓘ

7 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$
4	NAG	I	1	1,4	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	I	2	4	14,14,15	0.75	0	17,19,21	1.15	2 (11%)
4	MAN	I	3	4	11,11,12	2.17	4 (36%)	15,15,17	1.42	2 (13%)
5	NAG	J	1	5,1	14,14,15	0.94	1 (7%)	17,19,21	0.57	0
5	NAG	J	2	5	14,14,15	0.85	1 (7%)	17,19,21	0.80	0
5	MAN	J	3	5	11,11,12	2.11	4 (36%)	15,15,17	1.78	2 (13%)
5	BMA	J	4	5	11,11,12	1.79	4 (36%)	15,15,17	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	MAN	I	3	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	3/6/23/26	0/1/1/1
5	MAN	J	3	5	-	1/2/19/22	0/1/1/1
5	BMA	J	4	5	-	0/2/19/22	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	MAN	O5-C1	5.27	1.52	1.43
5	J	3	MAN	C2-C3	4.64	1.59	1.52
5	J	4	BMA	C4-C3	3.12	1.60	1.52
5	J	1	NAG	O5-C1	2.85	1.48	1.43
5	J	4	BMA	C2-C3	2.77	1.56	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	MAN	C1-O5-C5	5.24	119.21	112.19
4	I	3	MAN	C1-O5-C5	2.75	115.87	112.19
4	I	3	MAN	C1-C2-C3	2.74	113.63	109.64
5	J	3	MAN	C1-C2-C3	2.68	113.55	109.64
4	I	2	NAG	O4-C4-C5	-2.33	103.58	109.32

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

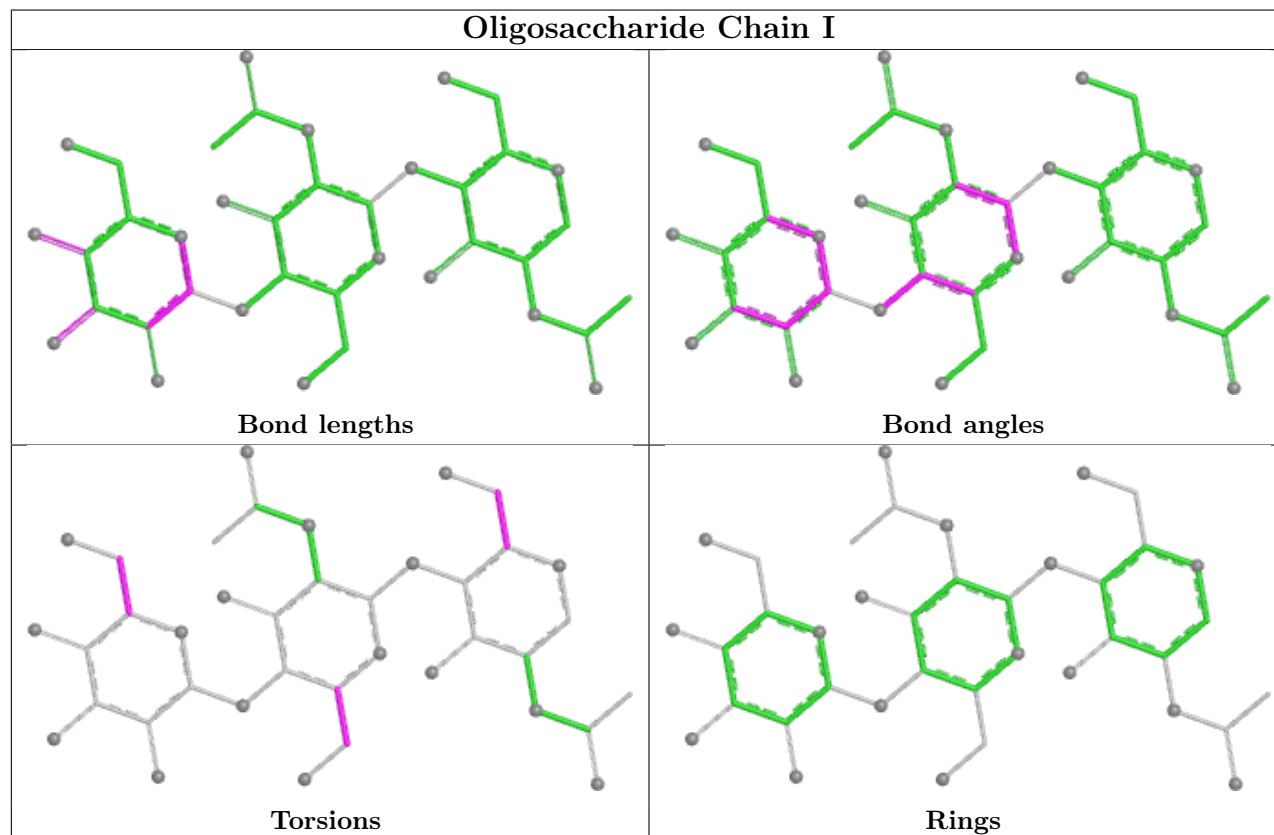
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0

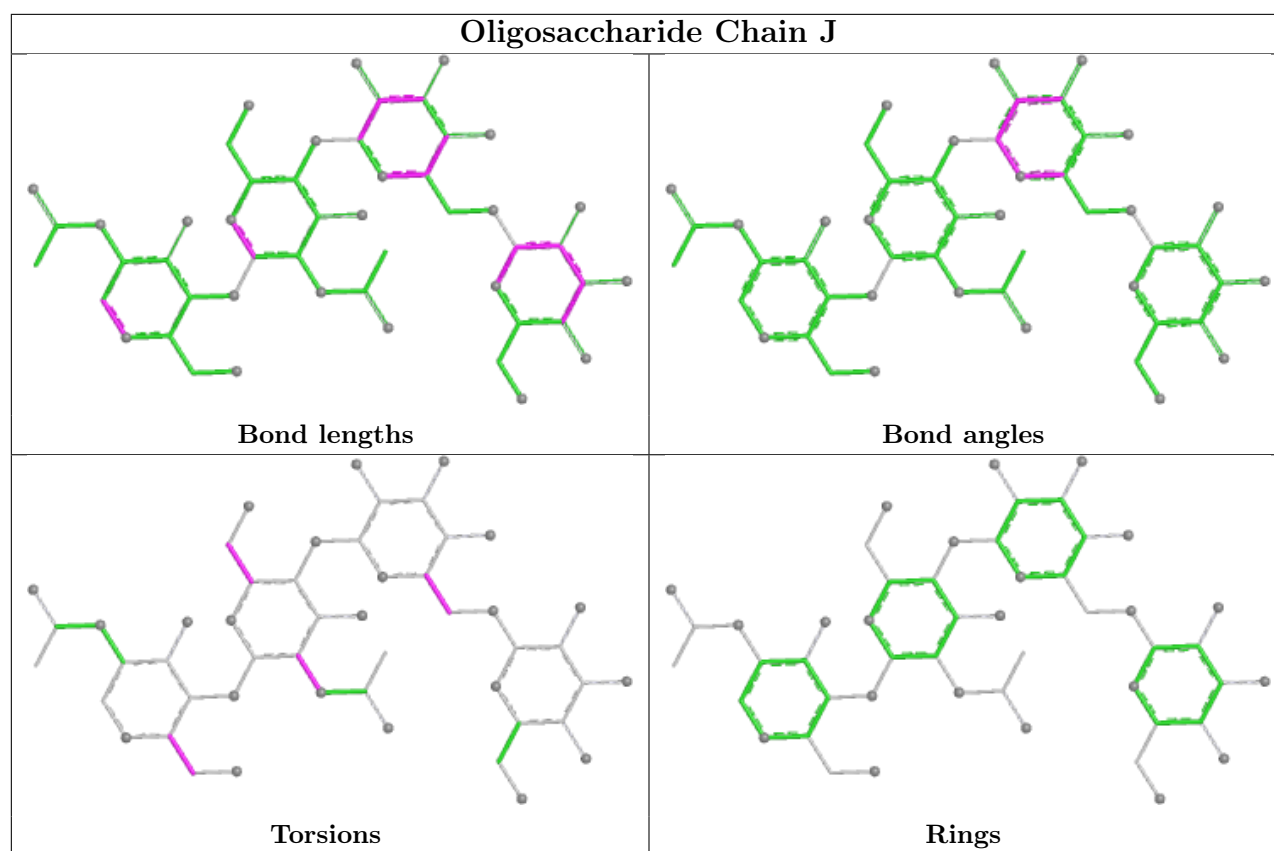
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2	NAG	1	0
5	J	4	BMA	1	0

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
6	GOL	E	1602	-	5,5,5	1.15	0	5,5,5	1.08	0
6	GOL	B	1601	-	5,5,5	1.78	2 (40%)	5,5,5	0.62	0
6	GOL	C	1601	-	5,5,5	0.95	0	5,5,5	1.06	0
9	NAG	E	1601	2	14,14,15	0.40	0	17,19,21	0.80	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
6	GOL	E	1602	-	-	2/4/4/4	-
6	GOL	B	1601	-	-	3/4/4/4	-
6	GOL	C	1601	-	-	0/4/4/4	-
9	NAG	E	1601	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1601	GOL	C3-C2	3.15	1.63	1.51
6	B	1601	GOL	C1-C2	2.23	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1601	NAG	C1-O5-C5	2.22	115.16	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1601	GOL	C1-C2-C3-O3
6	E	1602	GOL	O1-C1-C2-C3
6	E	1602	GOL	O1-C1-C2-O2
6	B	1601	GOL	O2-C2-C3-O3
6	B	1601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1602	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 [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	B	645/645 (100%)	-1.59	0 100 100	47, 108, 152, 185	0
1	C	645/645 (100%)	-1.60	0 100 100	57, 104, 150, 179	0
2	A	842/898 (93%)	-1.54	0 100 100	55, 127, 164, 192	0
2	E	504/898 (56%)	-1.59	0 100 100	58, 111, 170, 204	0
3	D	185/195 (94%)	-1.54	0 100 100	78, 108, 133, 155	0
3	H	185/195 (94%)	-1.62	0 100 100	68, 93, 123, 145	0
All	All	3006/3476 (86%)	-1.58	0 100 100	47, 111, 159, 204	0

There are no RSRZ outliers to report.

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

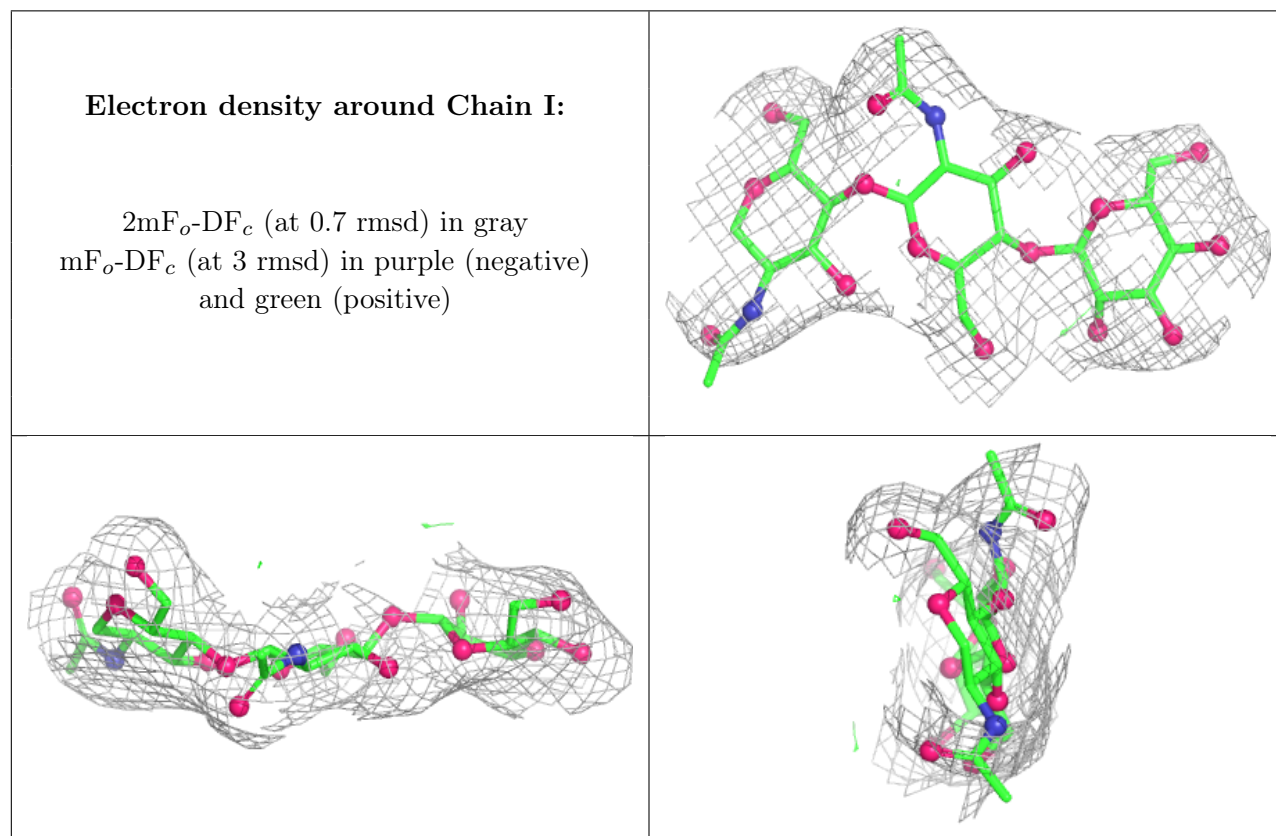
There are no non-standard protein/DNA/RNA residues in this entry.

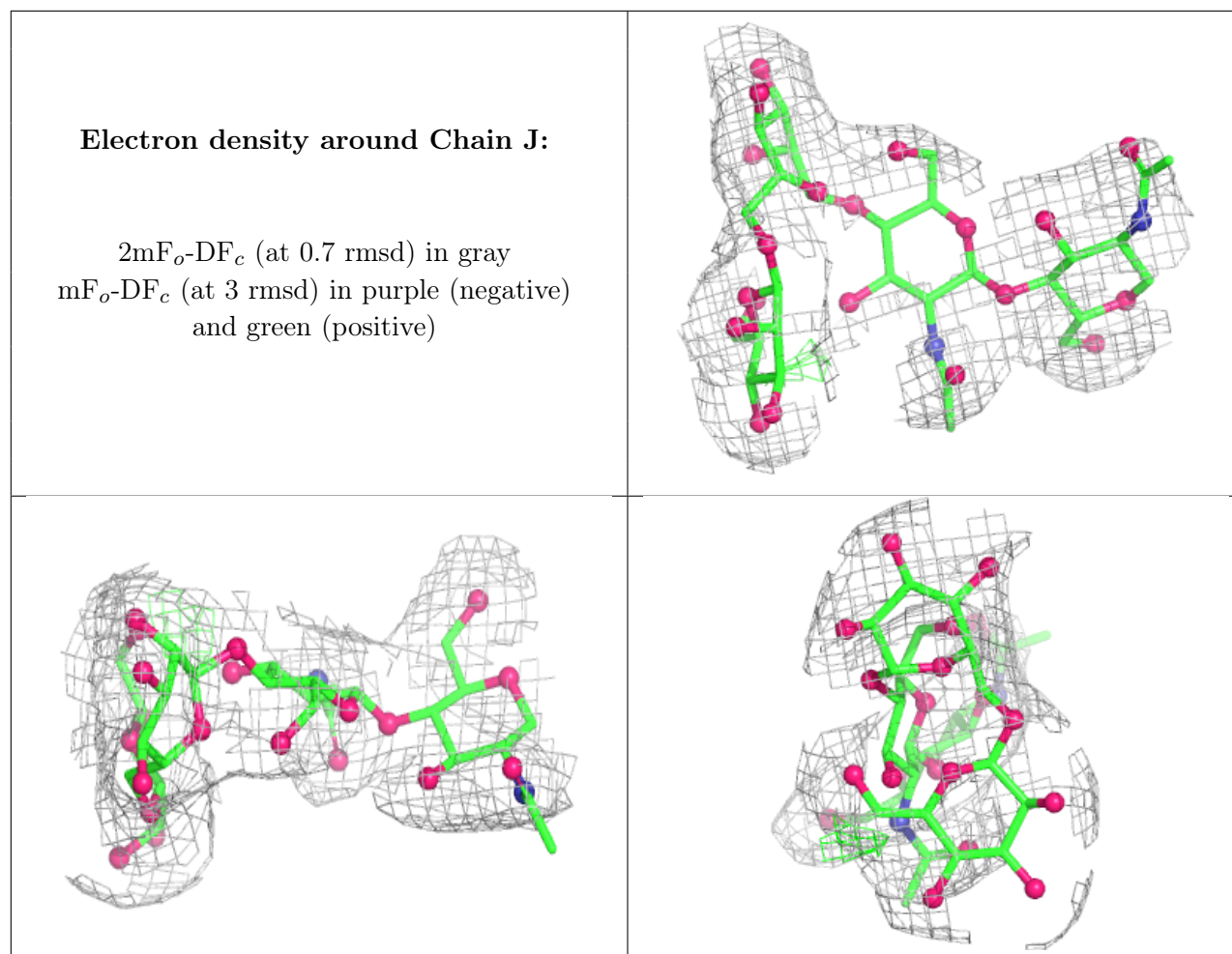
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
4	NAG	I	1	14/15	-	-	123,128,134,135	0
4	NAG	I	2	14/15	-	-	138,141,144,145	0
4	MAN	I	3	11/12	-	-	120,126,137,141	0
5	NAG	J	1	14/15	-	-	98,107,131,132	0
5	NAG	J	2	14/15	-	-	106,118,132,140	0
5	MAN	J	3	11/12	-	-	135,144,147,150	0
5	BMA	J	4	11/12	-	-	119,126,140,143	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
9	NAG	E	1601	14/15	0.96	0.05	157,161,166,168	0
6	GOL	C	1601	6/6	0.99	0.04	81,91,93,93	0
6	GOL	E	1602	6/6	0.99	0.08	69,73,75,76	0
8	MG	D	2101	1/1	0.99	0.02	117,117,117,117	0
8	MG	H	2001	1/1	0.99	0.03	82,82,82,82	0
6	GOL	B	1601	6/6	0.99	0.07	67,70,71,73	0
7	K	C	1602	1/1	1.00	0.03	71,71,71,71	0
7	K	A	1601	1/1	1.00	0.04	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.