Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 11:08 am GMT

PDB ID	:	7B26
Title	:	CirpA1 in complex with pseudo-monomeric Properdin lacking TSR2-3
Authors	:	Lea, S.M.; Johnson, S.; Braunger, K.
Deposited on	:	2020-11-26
Resolution	:	3.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

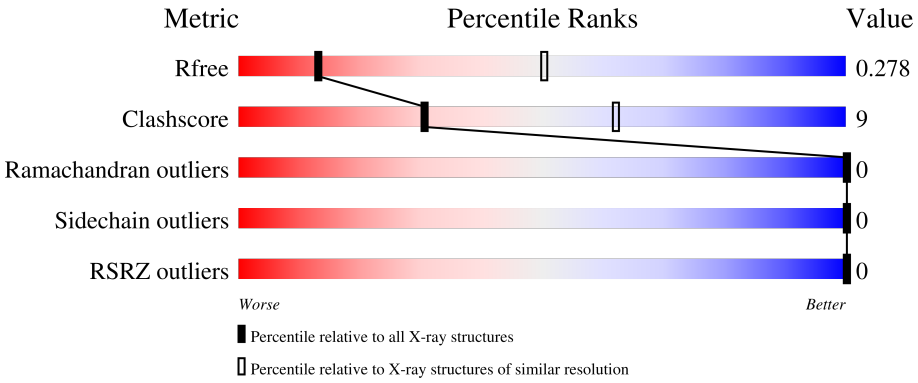
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	247	64% 13% 23%
2	A	134	61% 18% 21%
3	C	180	69% 17% 13%
4	D	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3684 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 Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	191	1498	926	283	268	21	0	1	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	229	MET	-	initiating methionine	UNP P27918
B	230	ILE	-	expression tag	UNP P27918
B	231	THR	-	expression tag	UNP P27918
B	232	GLU	-	expression tag	UNP P27918
B	233	GLY	-	expression tag	UNP P27918
B	234	ALA	-	expression tag	UNP P27918
B	235	GLN	-	expression tag	UNP P27918
B	236	ALA	-	expression tag	UNP P27918
B	237	PRO	-	expression tag	UNP P27918
B	238	ARG	-	expression tag	UNP P27918
B	239	LEU	-	expression tag	UNP P27918
B	240	LEU	-	expression tag	UNP P27918
B	241	LEU	-	expression tag	UNP P27918
B	242	PRO	-	expression tag	UNP P27918
B	243	PRO	-	expression tag	UNP P27918
B	244	LEU	-	expression tag	UNP P27918
B	245	LEU	-	expression tag	UNP P27918
B	246	LEU	-	expression tag	UNP P27918
B	247	LEU	-	expression tag	UNP P27918
B	248	LEU	-	expression tag	UNP P27918
B	249	THR	-	expression tag	UNP P27918
B	250	LEU	-	expression tag	UNP P27918
B	251	PRO	-	expression tag	UNP P27918
B	252	ALA	-	expression tag	UNP P27918
B	253	THR	-	expression tag	UNP P27918
B	254	GLY	-	expression tag	UNP P27918
B	255	SER	-	expression tag	UNP P27918

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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	HIS	-	expression tag	UNP P27918
B	471	HIS	-	expression tag	UNP P27918
B	472	HIS	-	expression tag	UNP P27918
B	473	HIS	-	expression tag	UNP P27918
B	474	HIS	-	expression tag	UNP P27918
B	475	HIS	-	expression tag	UNP P27918

- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	106	Total	C	N	O	S	0	0	0
			805	495	144	154	12			

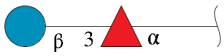
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	CYS	engineered mutation	UNP P27918

- Molecule 3 is a protein called CirpA1.

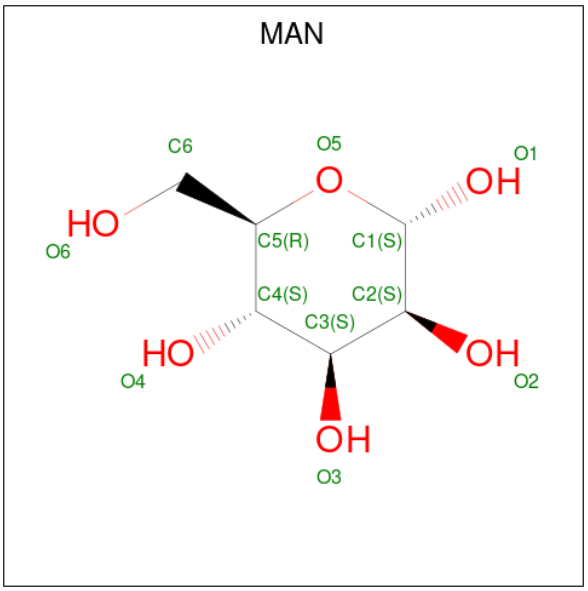
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1261	796	206	253	6			

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



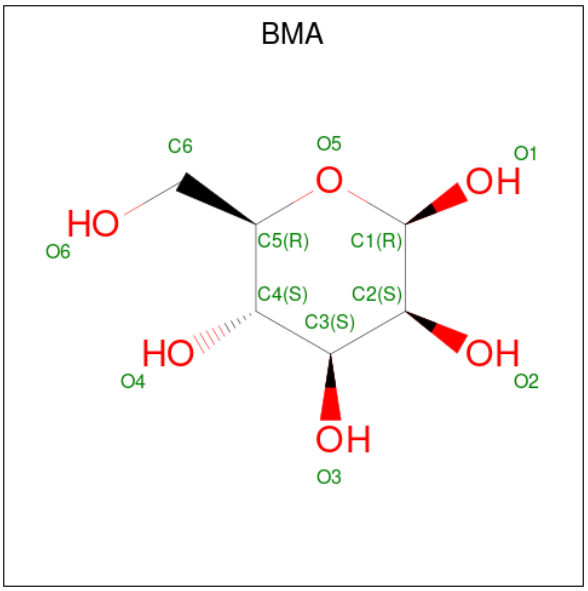
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



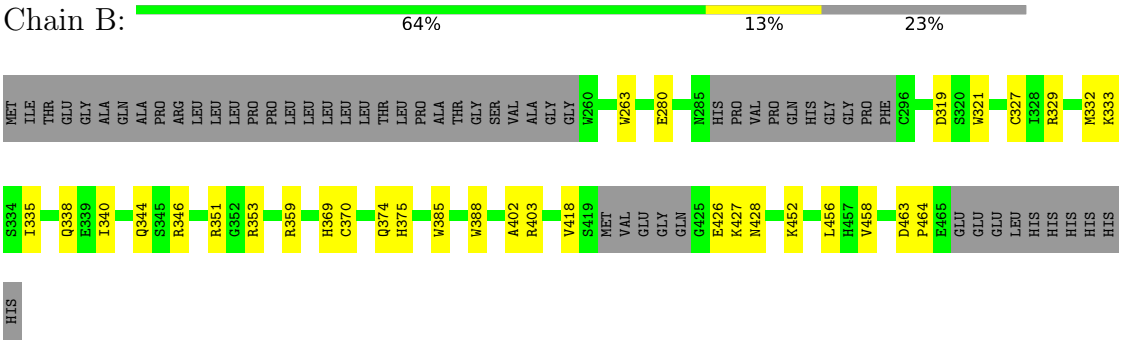
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 11 6 5	0	0

3 Residue-property plots (i)

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

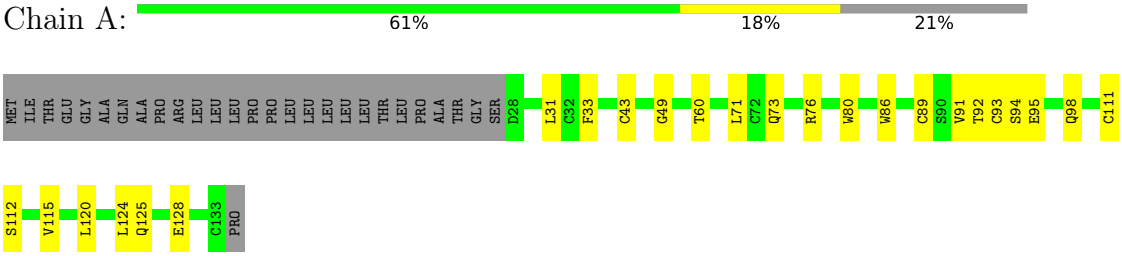
• Molecule 1: Properdin

Chain B:



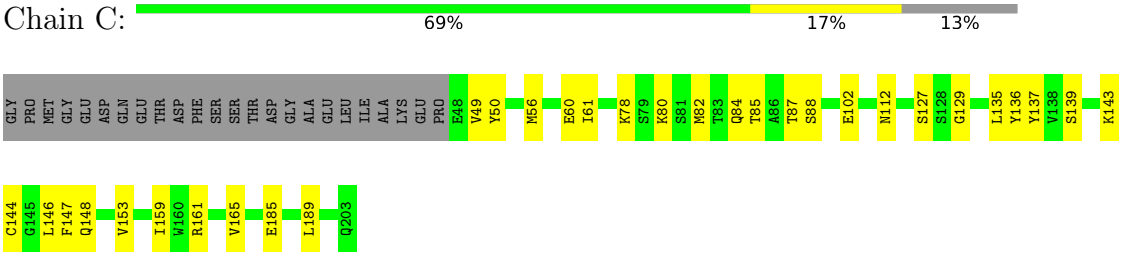
• Molecule 2: Properdin

Chain A:



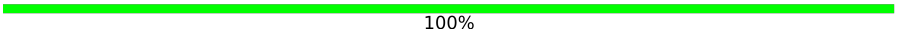
• Molecule 3: CirpA1

Chain C:



• Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain D:




FUC1
BGC2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.31Å 54.51Å 70.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.71 – 3.40 83.16 – 2.84	Depositor EDS
% Data completeness (in resolution range)	73.2 (24.71-3.40) 47.2 (83.16-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18rc4_3812	Depositor
R, R_{free}	0.229 , 0.274 0.229 , 0.278	Depositor DCC
R_{free} test set	364 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3684	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 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, MAN, BGC

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	0.30	0/1547	0.58	0/2104
2	A	0.31	0/824	0.56	0/1116
3	C	0.29	0/1291	0.52	0/1749
All	All	0.30	0/3662	0.55	0/4969

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1498	0	1425	30	0
2	A	805	0	748	16	0
3	C	1261	0	1195	27	0
4	D	21	0	19	0	0
5	A	22	0	20	0	0
5	B	66	0	60	0	0
6	B	11	0	10	0	0
All	All	3684	0	3477	66	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 (66) 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:B:418:VAL:HB	1:B:426:GLU:HA	1.57	0.83
3:C:84:GLN:HG2	3:C:85:THR:HG23	1.66	0.77
1:B:374:GLN:HG3	1:B:375:HIS:CD2	2.22	0.74
1:B:329:ARG:HB2	1:B:335:ILE:HD11	1.70	0.72
1:B:418:VAL:HG11	1:B:426:GLU:HB2	1.71	0.71
2:A:33:PHE:CG	2:A:43:CYS:HB3	2.33	0.64
1:B:456:LEU:HD11	2:A:95:GLU:O	1.96	0.64
2:A:89:CYS:HB3	2:A:98:GLN:HB3	1.77	0.64
3:C:139:SER:HB3	3:C:144:CYS:HB3	1.78	0.64
3:C:135:LEU:HD13	3:C:147:PHE:HE1	1.63	0.62
1:B:319:ASP:OD2	1:B:351:ARG:NH1	2.30	0.62
3:C:49:VAL:HG21	3:C:112:ASN:HD22	1.65	0.61
3:C:49:VAL:HG11	3:C:112:ASN:HB3	1.84	0.59
2:A:91:VAL:HG21	2:A:94:SER:O	2.03	0.59
3:C:129:GLY:HA3	3:C:153:VAL:HG22	1.84	0.58
3:C:135:LEU:HD13	3:C:147:PHE:CE1	2.37	0.58
1:B:418:VAL:CB	1:B:426:GLU:HA	2.31	0.57
2:A:60:THR:HG23	2:A:76:ARG:HA	1.86	0.56
1:B:344:GLN:HG3	1:B:370:CYS:SG	2.46	0.56
1:B:335:ILE:HG23	1:B:340:ILE:HB	1.88	0.56
3:C:102:GLU:OE2	3:C:127:SER:OG	2.20	0.55
3:C:129:GLY:HA3	3:C:153:VAL:CG2	2.36	0.55
1:B:329:ARG:CB	1:B:335:ILE:HD11	2.36	0.55
1:B:327:CYS:HB2	1:B:344:GLN:HE21	1.72	0.55
1:B:353:ARG:HD2	1:B:359:ARG:HA	1.88	0.55
2:A:94:SER:OG	2:A:95:GLU:N	2.40	0.55
1:B:329:ARG:NH2	3:C:185:GLU:OE2	2.37	0.55
1:B:402:ALA:HB2	1:B:452:LYS:HD3	1.89	0.54
1:B:463:ASP:OD1	1:B:464:PRO:HD2	2.07	0.54
2:A:71:LEU:HD21	2:A:73:GLN:HE21	1.73	0.54
2:A:95:GLU:HG2	2:A:128:GLU:OE2	2.08	0.53
3:C:148:GLN:OE1	3:C:161:ARG:NE	2.43	0.52
2:A:33:PHE:CD2	2:A:43:CYS:HB3	2.45	0.51
2:A:92:THR:HG23	2:A:93:CYS:H	1.76	0.51
1:B:458:VAL:HG22	2:A:124:LEU:HD21	1.93	0.50
3:C:136:TYR:CZ	3:C:146:LEU:HB3	2.47	0.50
1:B:340:ILE:HD12	3:C:189:LEU:HB3	1.92	0.50
3:C:60:GLU:HG2	3:C:78:LYS:HG2	1.93	0.50
3:C:82:MET:HG3	3:C:87:THR:HB	1.93	0.50
2:A:86:TRP:CH2	2:A:125:GLN:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:LYS:O	3:C:165:VAL:HA	2.13	0.49
1:B:418:VAL:HG12	1:B:427:LYS:H	1.79	0.47
1:B:263:TRP:CE3	1:B:280:GLU:HG3	2.49	0.47
1:B:385:TRP:CG	1:B:403:ARG:NH1	2.83	0.47
3:C:49:VAL:HG11	3:C:112:ASN:CB	2.45	0.46
2:A:111:CYS:HB2	2:A:115:VAL:CG1	2.46	0.45
3:C:56:MET:HA	3:C:61:ILE:HD11	1.97	0.45
1:B:463:ASP:OD1	2:A:120:LEU:HD11	2.15	0.45
3:C:50:TYR:CE2	3:C:137:TYR:HA	2.52	0.45
1:B:329:ARG:HB3	1:B:332:MET:HB3	1.99	0.44
3:C:49:VAL:HG21	3:C:112:ASN:ND2	2.31	0.44
1:B:388:TRP:CE2	1:B:403:ARG:HD3	2.53	0.43
1:B:418:VAL:HG11	1:B:426:GLU:CB	2.45	0.42
2:A:80:TRP:HE1	2:A:112:SER:HB2	1.84	0.42
1:B:374:GLN:HG3	1:B:375:HIS:HD2	1.76	0.42
1:B:333:LYS:HE2	3:C:137:TYR:HD1	1.84	0.42
1:B:321:TRP:HB3	1:B:346:ARG:HD2	2.01	0.41
1:B:369:HIS:HB2	1:B:428:ASN:O	2.21	0.41
3:C:80:LYS:HG2	3:C:88:SER:O	2.20	0.41
3:C:49:VAL:HG11	3:C:112:ASN:HD22	1.85	0.41
3:C:80:LYS:HE3	3:C:88:SER:HB3	2.01	0.41
1:B:319:ASP:CG	1:B:351:ARG:HH12	2.21	0.41
2:A:31:LEU:HD23	2:A:49:GLY:HA2	2.03	0.41
3:C:82:MET:HA	3:C:87:THR:HA	2.02	0.41
3:C:147:PHE:O	3:C:161:ARG:HA	2.21	0.40
1:B:338:GLN:OE1	3:C:159:ILE:HD12	2.22	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	B	186/247 (75%)	181 (97%)	5 (3%)	0	100	100
2	A	104/134 (78%)	95 (91%)	9 (9%)	0	100	100
3	C	154/180 (86%)	151 (98%)	3 (2%)	0	100	100
All	All	444/561 (79%)	427 (96%)	17 (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	B	168/212 (79%)	168 (100%)	0	100	100
2	A	88/111 (79%)	88 (100%)	0	100	100
3	C	144/163 (88%)	144 (100%)	0	100	100
All	All	400/486 (82%)	400 (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. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

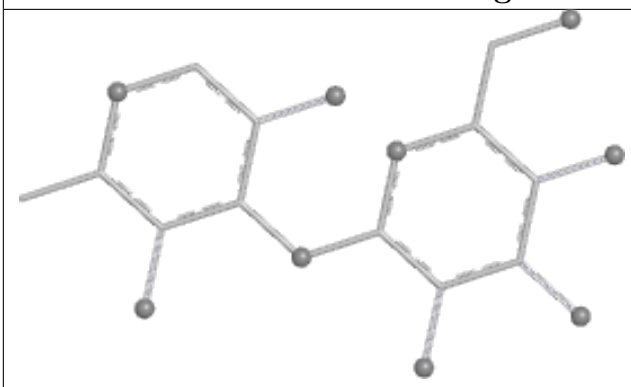
There are no torsion outliers.

There are no ring outliers.

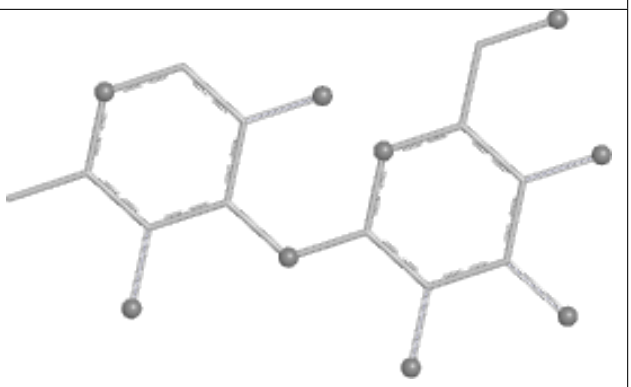
No monomer is involved in short contacts.

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

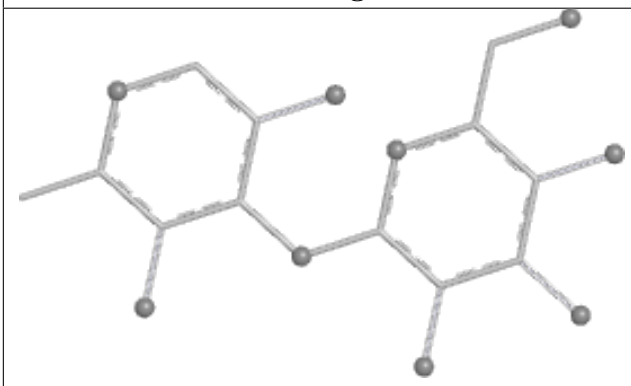
Oligosaccharide Chain D



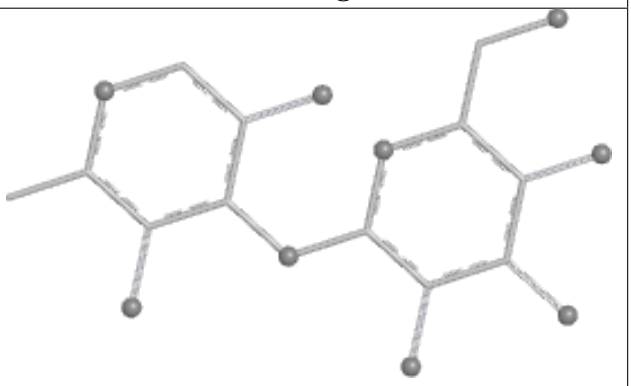
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	191/247 (77%)	-0.45	0	100	100	38, 67, 95, 118	0
2	A	106/134 (79%)	-0.46	0	100	100	36, 53, 141, 158	0
3	C	156/180 (86%)	-0.36	0	100	100	31, 66, 97, 108	0
All	All	453/561 (80%)	-0.42	0	100	100	31, 65, 98, 158	0

There are no RSRZ outliers to report.

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

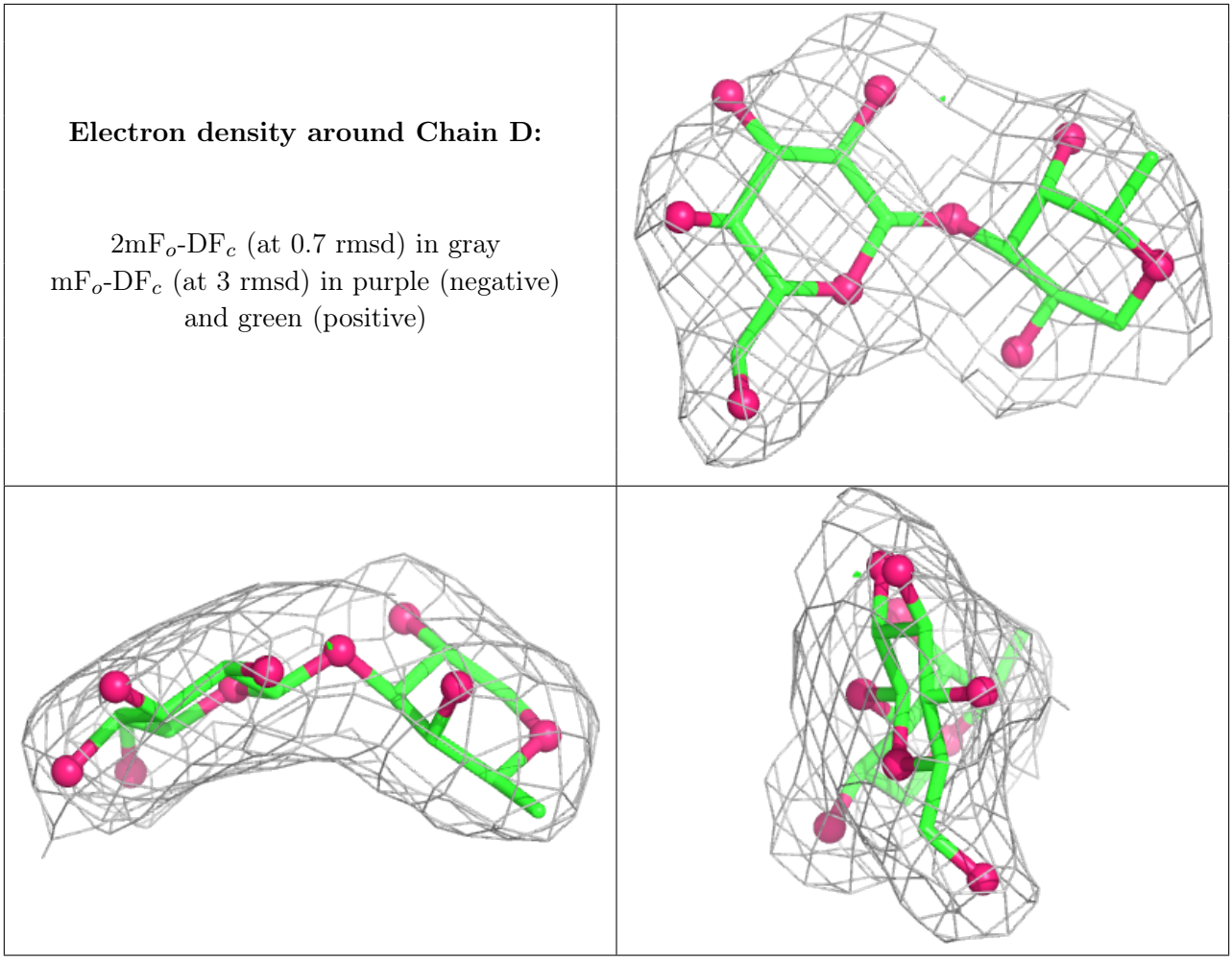
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BGC	D	2	11/12	0.94	0.14	27,33,44,62	0
4	FUC	D	1	10/11	0.97	0.13	27,41,42,42	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.

Electron density around Chain D:

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



6.4 Ligands

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, 95^{th} 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	MAN	A	201	11/12	0.83	0.48	84,108,117,124	0
5	MAN	B	505	11/12	0.92	0.19	49,61,82,95	0
5	MAN	B	502	11/12	0.94	0.18	33,51,58,61	0
5	MAN	B	507	11/12	0.94	0.16	63,67,70,80	0
5	MAN	A	200	11/12	0.94	0.14	47,55,60,63	0
5	MAN	B	504	11/12	0.94	0.09	61,72,84,85	0
6	BMA	B	506	11/12	0.94	0.17	53,59,72,88	0
5	MAN	B	501	11/12	0.95	0.15	43,49,52,54	0
5	MAN	B	503	11/12	0.95	0.15	59,68,81,92	0

6.5 Other polymers (i)

There are no such residues in this entry.