Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 02:39 AM EDT

PDB ID	:	3ASR
Title	:	Crystal structure of P domain from Norovirus Funabashi258 stain in the complex with Lewis-a
Authors	:	Kubota, T.; Kumagai, A.; Itoh, H.; Furukawa, S.; Narimatsu, H.; Wakita, T.; Ishii, K.; Takeda, N.; Someya, Y.; Shirato, H.
Deposited on	:	2010-12-17
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

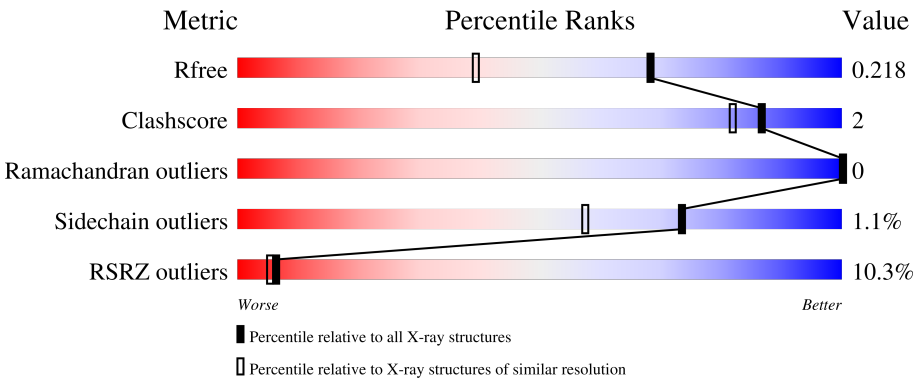
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	A	326	9%, 90%, 5%, 5%
1	B	326	10%, 85%, 7%, 7%
2	C	3	67%, 33%
2	D	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NPO	B	1001	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5218 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.

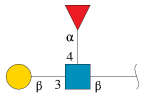
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2387	1527	402	449	9	0	1	0
1	B	302	2322	1488	391	434	9	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	GLY	-	expression tag	UNP Q8JW44
A	217	PRO	-	expression tag	UNP Q8JW44
A	218	LEU	-	expression tag	UNP Q8JW44
A	219	GLY	-	expression tag	UNP Q8JW44
A	220	SER	-	expression tag	UNP Q8JW44
B	216	GLY	-	expression tag	UNP Q8JW44
B	217	PRO	-	expression tag	UNP Q8JW44
B	218	LEU	-	expression tag	UNP Q8JW44
B	219	GLY	-	expression tag	UNP Q8JW44
B	220	SER	-	expression tag	UNP Q8JW44

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.

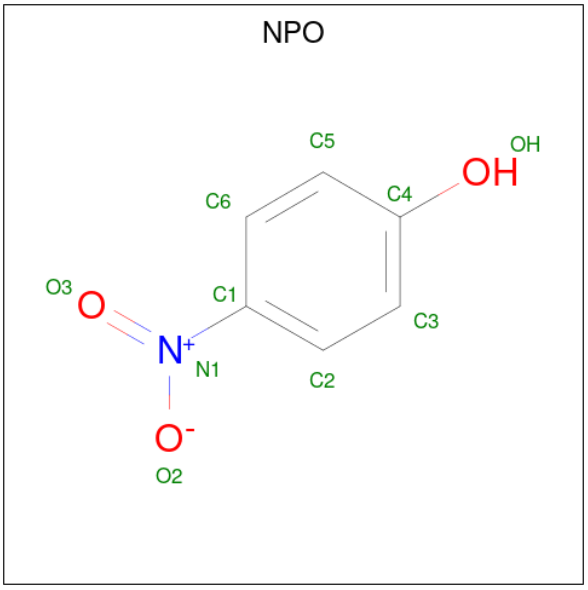


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	36	20	1	15	0	0	0
2	D	3	35	20	1	14	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0

- Molecule 4 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 10 6 1 3	0	0

- Molecule 5 is water.

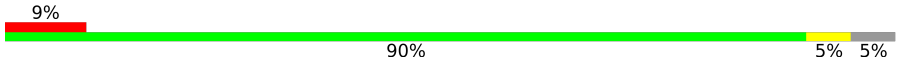
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	224	Total O 224 224	0	0
5	B	202	Total O 202 202	0	0

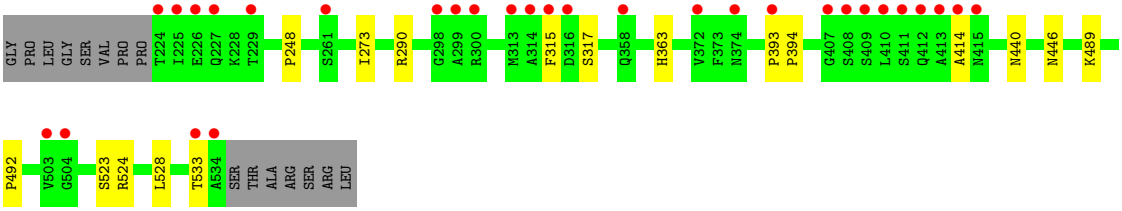
3 Residue-property plots (i)

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: Capsid protein

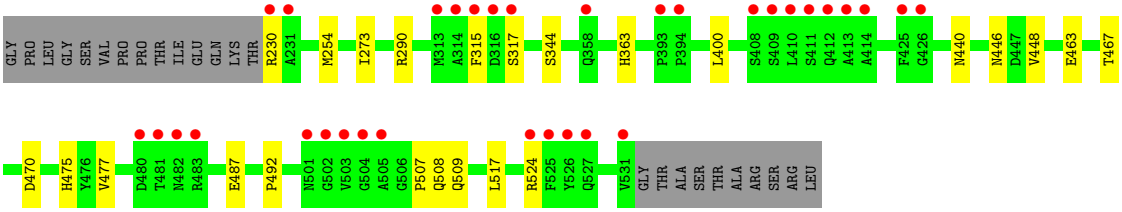
Chain A:





• Molecule 1: Capsid protein

Chain B:

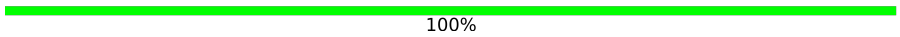


• Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	74.73Å 74.73Å 107.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.25 – 1.60 31.25 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (31.25-1.60) 98.6 (31.25-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.201 , 0.218 0.197 , 0.218	Depositor DCC
R_{free} test set	4398 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l 0.045 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, GAL, NPO, NAG, NA

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	0.37	0/2463	0.52	0/3372
1	B	0.37	0/2398	0.52	0/3284
All	All	0.37	0/4861	0.52	0/6656

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 (i)

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	2387	0	2316	7	0
1	B	2322	0	2249	14	0
2	C	36	0	33	1	0
2	D	35	0	31	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	10	0	4	0	0
5	A	224	0	0	0	0
5	B	202	0	0	0	0
All	All	5218	0	4633	20	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 2.

All (20) 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:248:PRO:O	1:B:290:ARG:NH2	2.27	0.67
1:B:254:MET:HG2	1:B:507:PRO:HB2	1.79	0.64
1:B:440:ASN:HD22	1:B:446:ASN:ND2	2.02	0.58
1:B:467:THR:HG21	1:B:492:PRO:HG3	1.86	0.58
1:B:400:LEU:HD13	1:B:448:VAL:HG22	1.86	0.57
1:A:315:PHE:HA	1:A:363:HIS:CE1	2.40	0.57
1:B:477:VAL:HG21	1:B:517:LEU:HD12	1.88	0.55
1:B:508:GLN:HG2	1:B:509:GLN:HE21	1.72	0.55
1:A:440:ASN:HD22	1:A:446:ASN:ND2	2.06	0.54
1:B:230:ARG:HD3	1:B:463:GLU:OE1	2.08	0.53
1:A:363:HIS:CE1	1:A:414:ALA:H	2.28	0.52
1:B:470:ASP:HB2	1:B:524:ARG:N	2.25	0.50
1:A:273:ILE:HG12	1:A:492:PRO:HA	1.94	0.48
1:B:273:ILE:HG12	1:B:492:PRO:HA	1.97	0.46
1:B:470:ASP:HB3	1:B:524:ARG:HB3	1.99	0.43
1:B:344:SER:HB2	2:C:3:FUC:H2	2.00	0.43
1:A:393:PRO:HA	1:A:394:PRO:HD3	1.92	0.41
1:B:315:PHE:HA	1:B:363:HIS:NE2	2.35	0.41
1:A:489:LYS:HG3	1:A:528:LEU:HD21	2.03	0.41
1:B:475:HIS:CD2	1:B:487:GLU:HG2	2.57	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	310/326 (95%)	307 (99%)	3 (1%)	0	100	100
1	B	301/326 (92%)	297 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	611/652 (94%)	604 (99%)	7 (1%)	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	266/277 (96%)	261 (98%)	5 (2%)	57	34
1	B	259/277 (94%)	258 (100%)	1 (0%)	91	84
All	All	525/554 (95%)	519 (99%)	6 (1%)	73	57

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ARG
1	A	317	SER
1	A	523	SER
1	A	524	ARG
1	A	533	THR
1	B	317	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	363	HIS
1	A	374	ASN
1	A	415	ASN
1	A	446	ASN
1	A	527	GLN
1	B	296	ASN
1	B	374	ASN
1	B	415	ASN

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Mol	Chain	Res	Type
1	B	446	ASN
1	B	509	GLN

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)

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	C	1	2	15,15,15	0.41	0	21,21,21	0.74	0
2	GAL	C	2	2	11,11,12	0.54	0	15,15,17	0.83	0
2	FUC	C	3	2	10,10,11	0.64	0	14,14,16	0.90	1 (7%)
2	NAG	D	1	2,4	14,14,15	0.50	0	17,19,21	0.76	0
2	GAL	D	2	2	11,11,12	0.49	0	15,15,17	0.79	0
2	FUC	D	3	2	10,10,11	0.54	0	14,14,16	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	0/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	FUC	C1-C2-C3	2.03	112.16	109.67

There are no chirality outliers.

There are no torsion outliers.

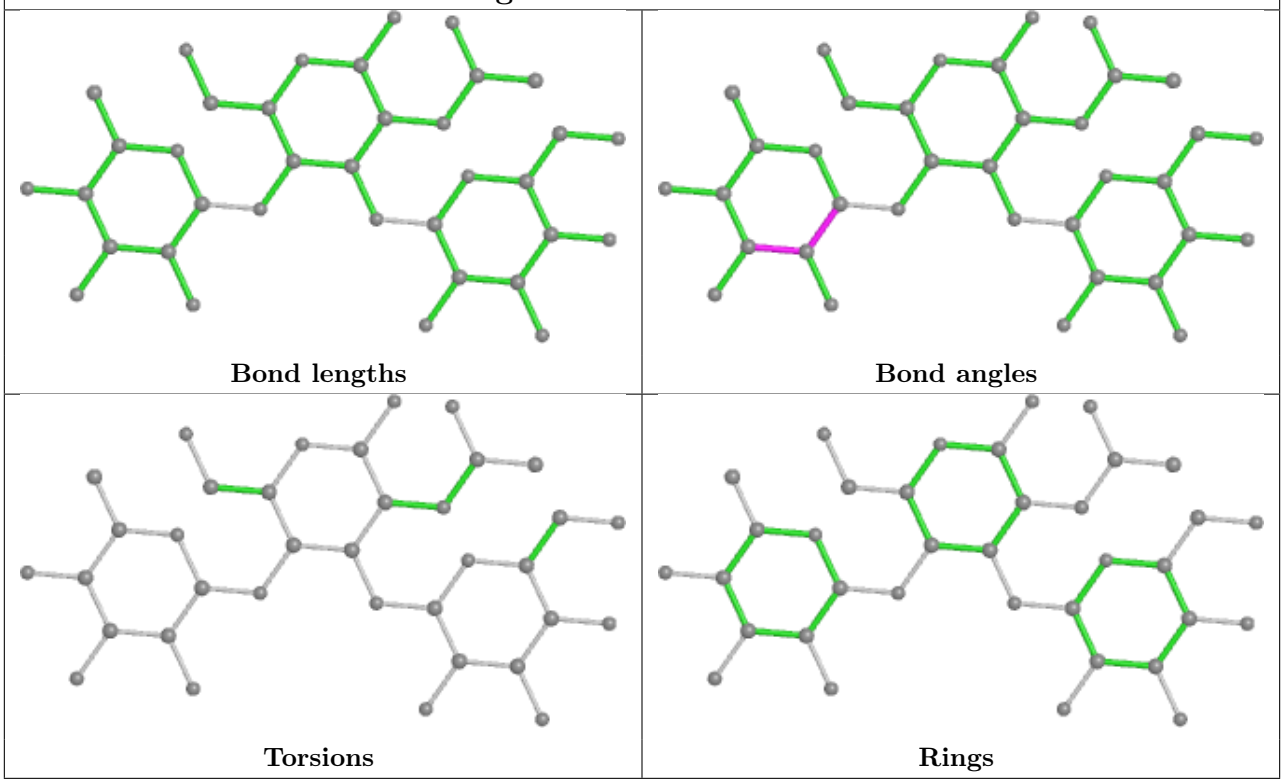
There are no ring outliers.

1 monomer is involved in 1 short contact:

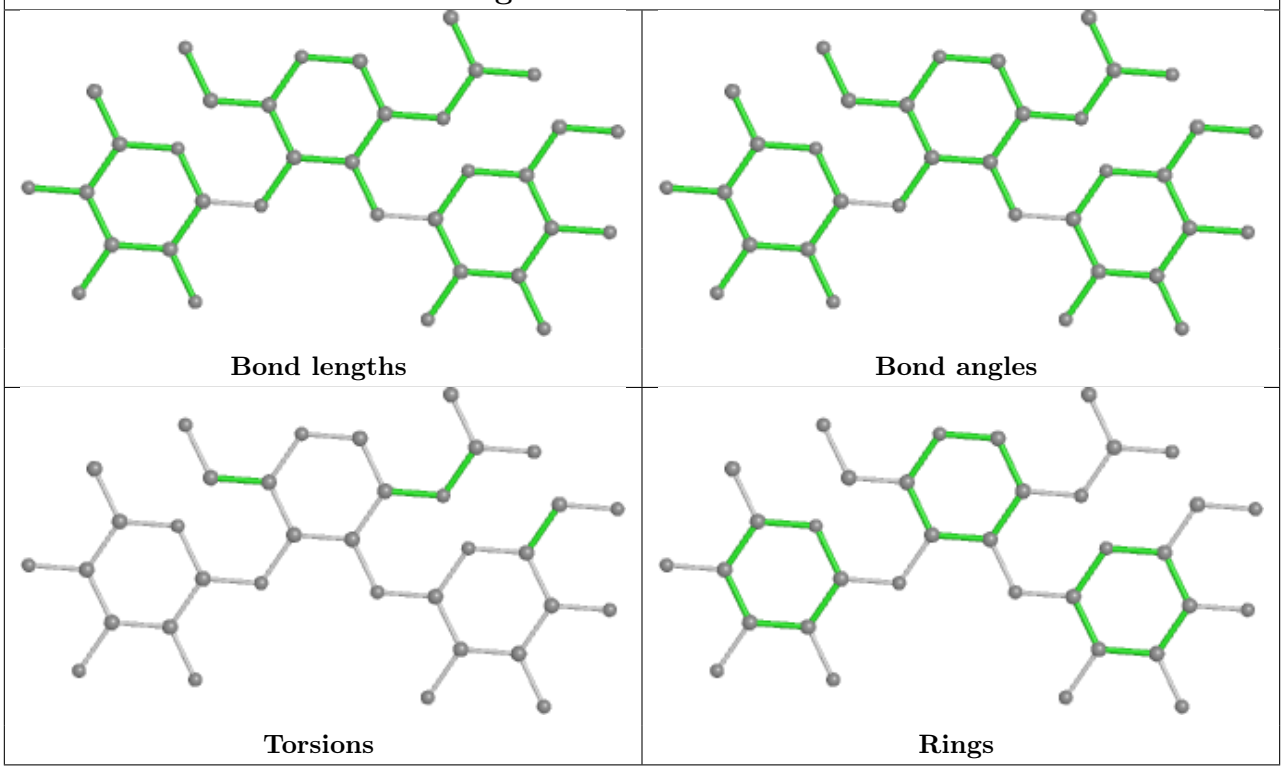
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FUC	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	NPO	B	1001	2	9,10,10	0.77	0	11,13,13	0.46	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	NPO	B	1001	2	-	2/2/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	NPO	C2-C1-N1-O3
4	B	1001	NPO	C6-C1-N1-O3

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 (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	311/326 (95%)	0.67	30 (9%)	8	7	16, 25, 39, 47	0
1	B	302/326 (92%)	0.69	33 (10%)	5	4	17, 25, 40, 45	0
All	All	613/652 (94%)	0.68	63 (10%)	6	5	16, 25, 40, 47	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	LEU	14.1
1	A	225	ILE	12.9
1	A	315	PHE	12.7
1	B	503	VAL	11.8
1	B	315	PHE	11.1
1	B	410	LEU	9.9
1	B	525	PHE	9.0
1	A	224	THR	9.0
1	B	409	SER	8.7
1	A	409	SER	8.3
1	A	534	ALA	7.4
1	B	231	ALA	7.1
1	B	314	ALA	7.0
1	A	411	SER	6.9
1	B	412	GLN	6.6
1	B	504	GLY	6.5
1	A	503	VAL	6.5
1	A	314	ALA	6.4
1	B	425	PHE	6.2
1	A	316	ASP	5.7
1	A	412	GLN	5.7
1	A	229	THR	5.6
1	B	524	ARG	5.2
1	B	502	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	504	GLY	5.1
1	B	313	MET	5.0
1	B	230	ARG	4.8
1	A	414	ALA	4.7
1	A	408	SER	4.5
1	A	226	GLU	4.4
1	B	483	ARG	4.1
1	A	227	GLN	4.1
1	B	501	ASN	4.1
1	A	374	ASN	4.0
1	B	411	SER	4.0
1	A	533	THR	3.9
1	B	481	THR	3.9
1	B	480	ASP	3.8
1	A	313	MET	3.6
1	A	413	ALA	3.5
1	B	408	SER	3.4
1	B	482	ASN	3.4
1	B	393	PRO	3.3
1	B	316	ASP	3.1
1	B	527	GLN	3.1
1	A	358	GLN	2.9
1	B	317	SER	2.8
1	A	372	VAL	2.8
1	B	505	ALA	2.7
1	A	261	SER	2.7
1	B	531	VAL	2.6
1	A	415	ASN	2.5
1	A	298	GLY	2.4
1	A	300	ARG	2.4
1	B	358	GLN	2.4
1	A	299	ALA	2.4
1	B	394	PRO	2.3
1	B	413	ALA	2.2
1	A	407	GLY	2.2
1	B	426	GLY	2.2
1	A	393	PRO	2.1
1	B	414	ALA	2.1
1	B	526	TYR	2.1

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)

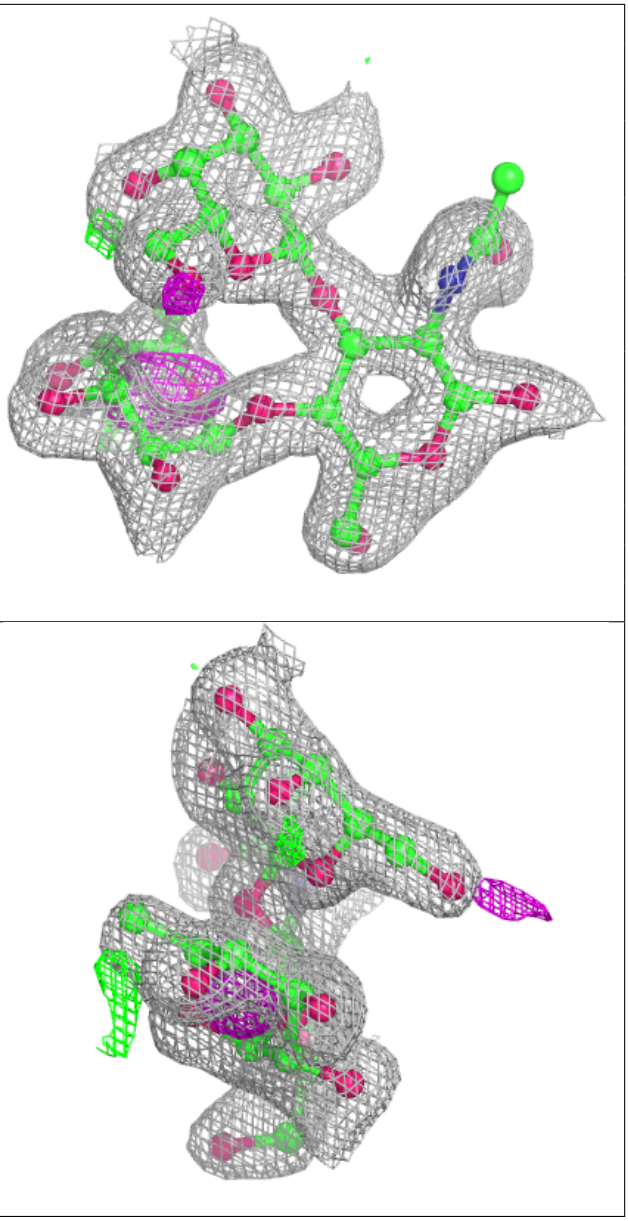
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	D	3	10/11	0.60	0.28	30,31,32,32	0
2	FUC	C	3	10/11	0.68	0.15	38,39,40,41	0
2	GAL	C	2	11/12	0.73	0.17	37,38,39,40	0
2	NAG	C	1	15/15	0.77	0.20	40,42,44,44	0
2	NAG	D	1	14/15	0.86	0.26	31,35,37,37	0
2	GAL	D	2	11/12	0.87	0.15	25,27,30,31	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.

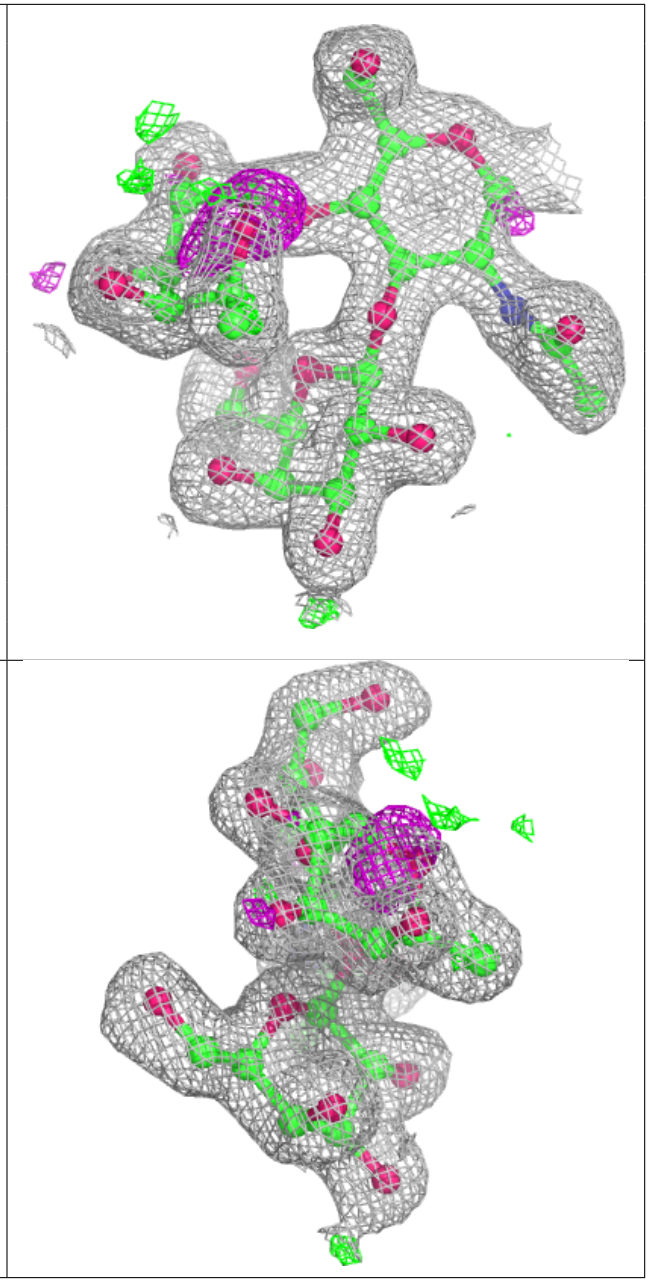
Electron density around Chain C:

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



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 (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	NPO	B	1001	10/10	0.63	0.41	43,47,50,50	0
3	NA	A	701	1/1	0.94	0.12	35,35,35,35	0
3	NA	B	701	1/1	0.99	0.15	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.