wwPDB X-ray Structure Validation Summary Report (i)

Oct 13, 2024 – 02:18 am BST

PDB ID	:	1E2S
Title	:	Crystal structure of an Arylsulfatase A mutant C69A
Authors	:	von Buelow, R.; Schmidt, B.; Dierks, T.; von Figura, K.; Uson, I.
Deposited on	:	2000-05-24
Resolution	:	2.35 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 (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:

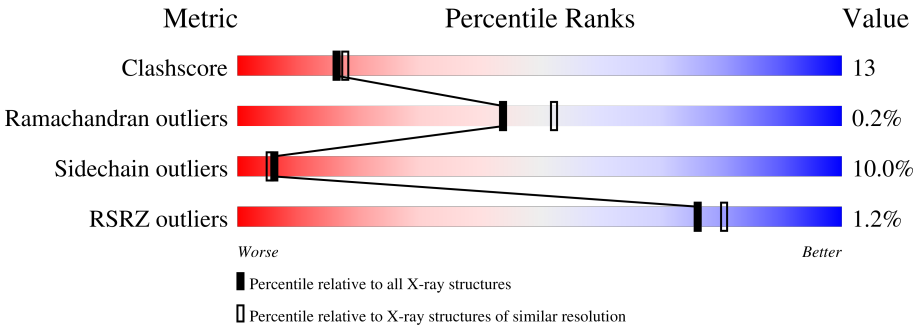
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.35 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))
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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 <=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	P	489	% 65% 25% 6%
2	A	2	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
2	NAG	A	1	X	-	-	-
2	NAG	A	2	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3773 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 Arylsulfatase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	P	481	3553	2270	603	657	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	69	ALA	CYS	engineered mutation	UNP P15289

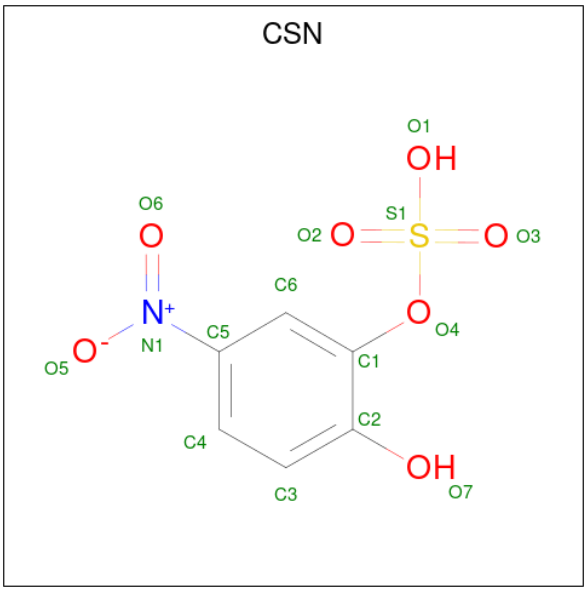
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	P	1	1	1	0	0

- Molecule 4 is N,4-DIHYDROXY-N-OXO-3-(SULFOOXY)BENZENAMINIUM (three-letter code: CSN) (formula: $C_6H_5NO_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	P	1	Total	C	N	O	S	0	1
			25	12	2	10	1		

- Molecule 5 is water.

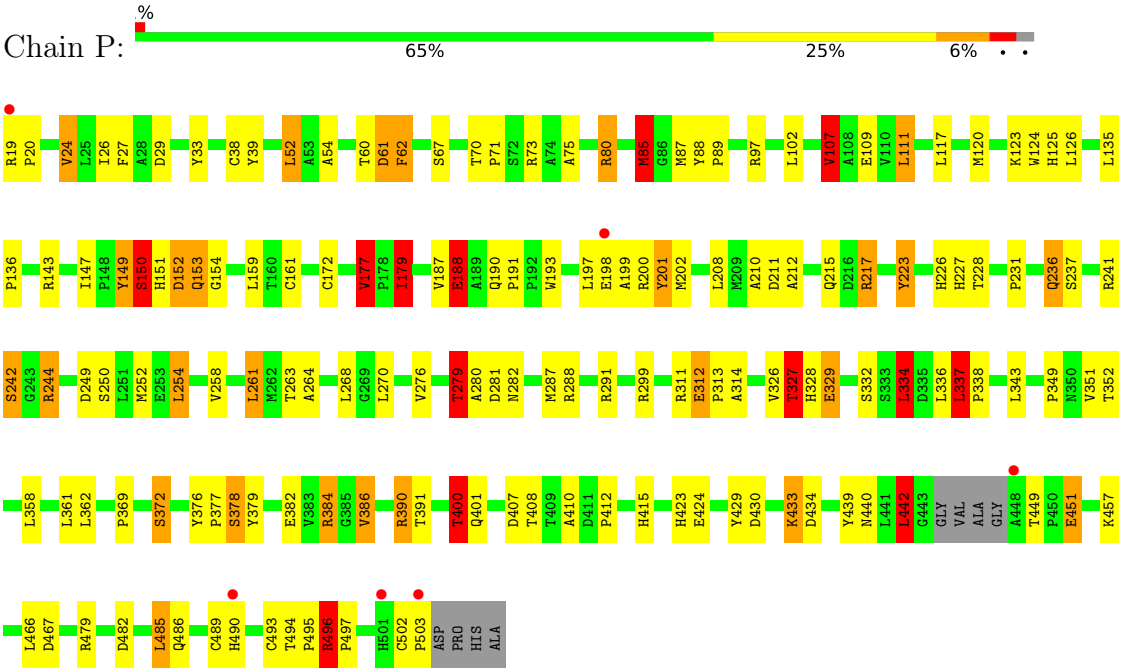
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	166	Total	O	0	0
			166	166		

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.

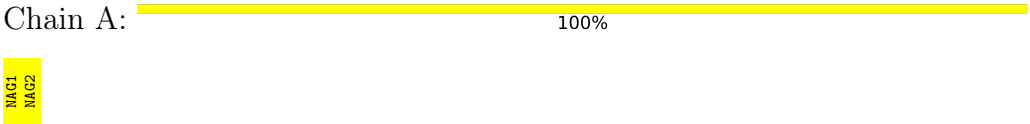
• Molecule 1: Arylsulfatase A

Chain P:



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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.80Å 131.80Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35 40.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.35) 99.2 (40.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.236 0.165 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.005 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3773	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: NAG, CSN, MG

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	P	0.93	2/3660 (0.1%)	1.89	97/5003 (1.9%)

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	P	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	503	PRO	N-CD	6.04	1.56	1.47
1	P	150	SER	CA-CB	5.01	1.60	1.52

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	291	ARG	NE-CZ-NH1	18.46	129.53	120.30
1	P	291	ARG	NE-CZ-NH2	-17.82	111.39	120.30
1	P	80	ARG	NE-CZ-NH2	14.62	127.61	120.30
1	P	33	TYR	CB-CG-CD1	-14.46	112.33	121.00
1	P	299	ARG	NE-CZ-NH1	-14.05	113.28	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	107	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	P	223	TYR	Mainchain
1	P	241	ARG	Mainchain
1	P	327	THR	Mainchain
1	P	54	ALA	Mainchain

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	P	3553	0	3421	88	1
2	A	28	0	25	0	0
3	P	1	0	0	0	0
4	P	25	0	6	2	0
5	P	166	0	0	17	0
All	All	3773	0	3452	90	1

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 13.

The worst 5 of 90 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:P:423:HIS:HD2	5:P:2140:HOH:O	1.50	0.93
1:P:109:GLU:OE2	5:P:2038:HOH:O	1.92	0.87
1:P:109:GLU:CD	5:P:2038:HOH:O	2.16	0.84
1:P:386:VAL:HG11	1:P:466:LEU:HD23	1.60	0.82
1:P:109:GLU:OE1	5:P:2038:HOH:O	1.99	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:490:HIS:NE2	1:P:490:HIS:NE2[16_554]	2.10	0.10

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	P	477/489 (98%)	446 (94%)	30 (6%)	1 (0%)	44 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS

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	P	369/384 (96%)	332 (90%)	37 (10%)	6 5

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	377	PRO
1	P	485	LEU
1	P	382	GLU
1	P	442	LEU
1	P	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	423	HIS
1	P	440	ASN
1	P	465	GLN
1	P	226	HIS
1	P	153	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)

2 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	A	1	2,1	14,14,15	1.72	4 (28%)	17,19,21	3.76	10 (58%)
2	NAG	A	2	2	14,14,15	1.41	2 (14%)	17,19,21	2.02	4 (23%)

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	A	1	2,1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	2	2	1/1/5/7	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAG	O7-C7	-3.35	1.15	1.23
2	A	1	NAG	O7-C7	-3.30	1.15	1.23
2	A	1	NAG	C2-N2	3.03	1.51	1.46
2	A	1	NAG	O5-C5	-2.71	1.38	1.43
2	A	2	NAG	C2-N2	2.59	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAG	C8-C7-N2	7.29	128.45	116.10
2	A	1	NAG	O7-C7-N2	-7.15	108.80	121.95
2	A	1	NAG	O4-C4-C3	6.15	124.57	110.35
2	A	2	NAG	C1-O5-C5	5.85	120.11	112.19
2	A	1	NAG	O5-C1-C2	5.50	119.98	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	NAG	C1
2	A	2	NAG	C1

All (4) torsion outliers are listed below:

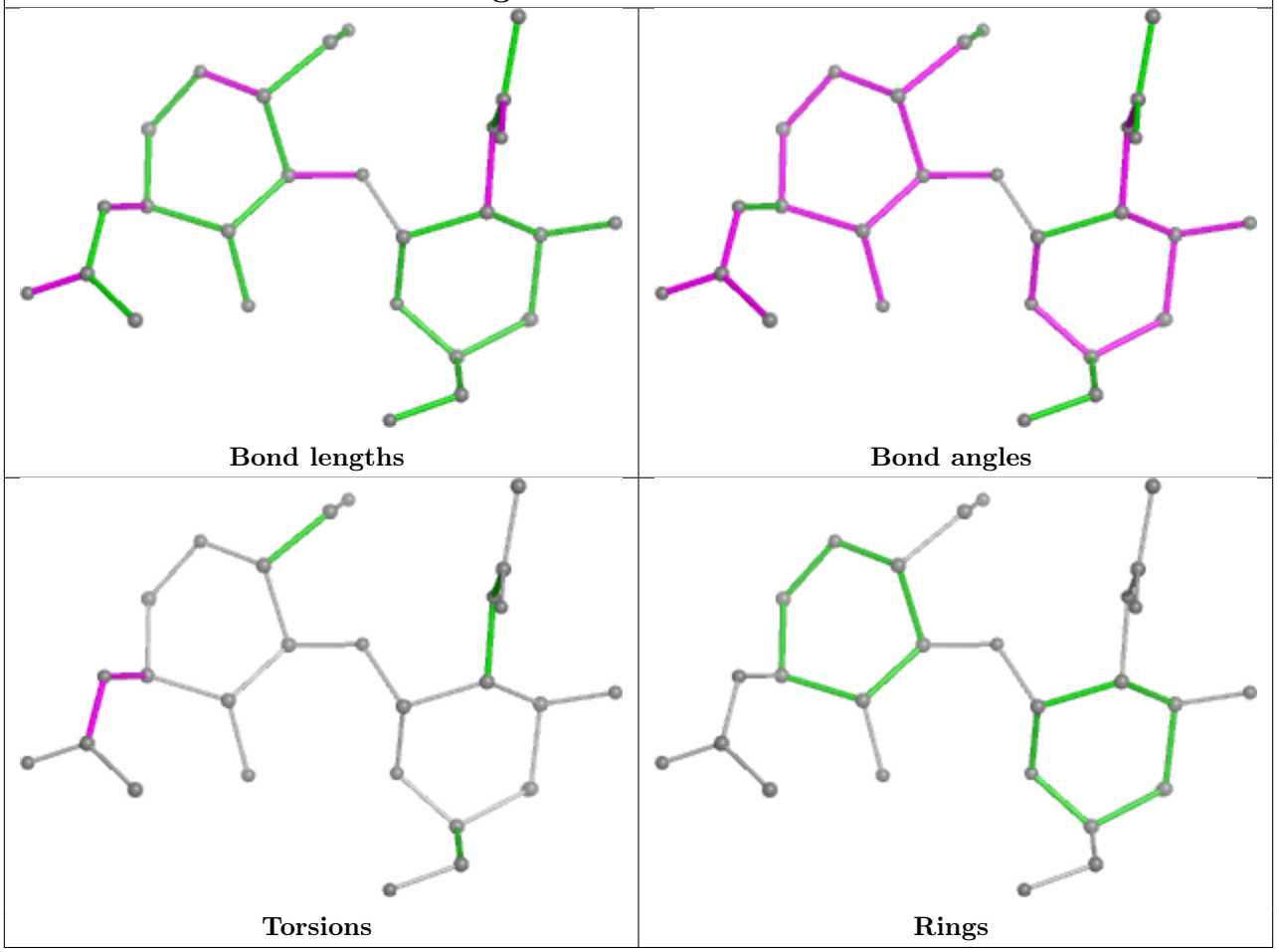
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	A	1	NAG	C1-C2-N2-C7
2	A	1	NAG	C3-C2-N2-C7

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 A



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	CSN	P	701[A]	-	14,15,15	1.48	3 (21%)	19,22,22	3.95	11 (57%)
4	CSN	P	701[B]	-	14,15,15	1.47	2 (14%)	19,22,22	2.62	12 (63%)

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	CSN	P	701[A]	-	-	2/7/9/9	0/1/1/1
4	CSN	P	701[B]	-	-	0/7/9/9	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	701[B]	CSN	O7-C2	-3.68	1.28	1.36
4	P	701[A]	CSN	O4-S1	3.56	1.63	1.58
4	P	701[B]	CSN	O4-S1	3.56	1.63	1.58
4	P	701[A]	CSN	O7-C2	-3.00	1.30	1.36
4	P	701[A]	CSN	O4-C1	-2.45	1.37	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	701[A]	CSN	C4-C5-N1	11.42	127.97	119.38
4	P	701[A]	CSN	C6-C5-N1	-6.46	113.05	118.75
4	P	701[A]	CSN	C3-C2-C1	-5.99	112.57	119.53
4	P	701[A]	CSN	C6-C1-C2	5.15	125.61	120.06
4	P	701[B]	CSN	C6-C5-N1	-4.56	114.72	118.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	701[A]	CSN	C2-C1-O4-S1
4	P	701[A]	CSN	C6-C1-O4-S1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	701[A]	CSN	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	P	481/489 (98%)	-0.12	6 (1%)	76 80	23, 40, 65, 86	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	448	ALA	6.7
1	P	503	PRO	4.9
1	P	198	GLU	4.5
1	P	490	HIS	3.8
1	P	19	ARG	2.2

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

SUGAR-RSR INFOmissingINFO

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
4	CSN	P	701[A]	15/15	0.91	0.22	53,64,69,72	10
4	CSN	P	701[B]	15/15	0.91	0.22	53,64,72,73	10
3	MG	P	600	1/1	0.98	0.04	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.