Full wwPDB X-ray Structure Validation Report (i)

Nov 28, 2023 – 07:31 pm GMT

PDB ID	:	1E1Z
Title	:	Crystal structure of an Arylsulfatase A mutant C69S
Authors	:	von Buelow, R.; Schmidt, B.; Dierks, T.; von Figura, K.; Uson, I.
Deposited on	:	2000-05-12
Resolution	:	2.40 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 (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:

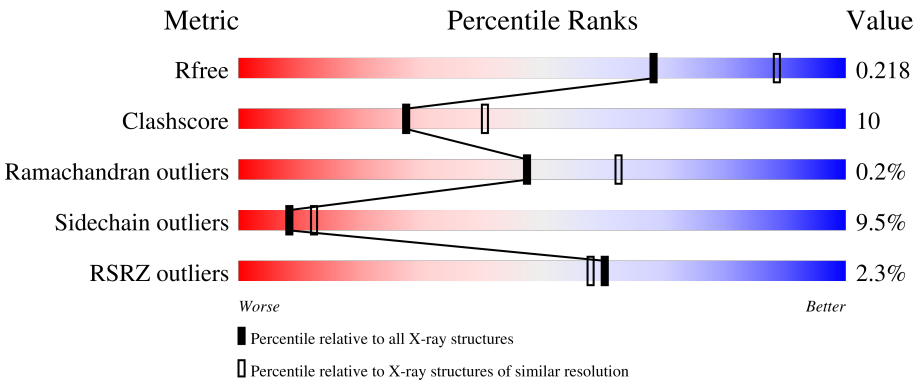
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	2% 66% 25% 6% • •
2	A	2	50% 50%

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 4 unique types of molecules in this entry. The entry contains 3740 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	3540	2263	599	655	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	69	SER	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 water.

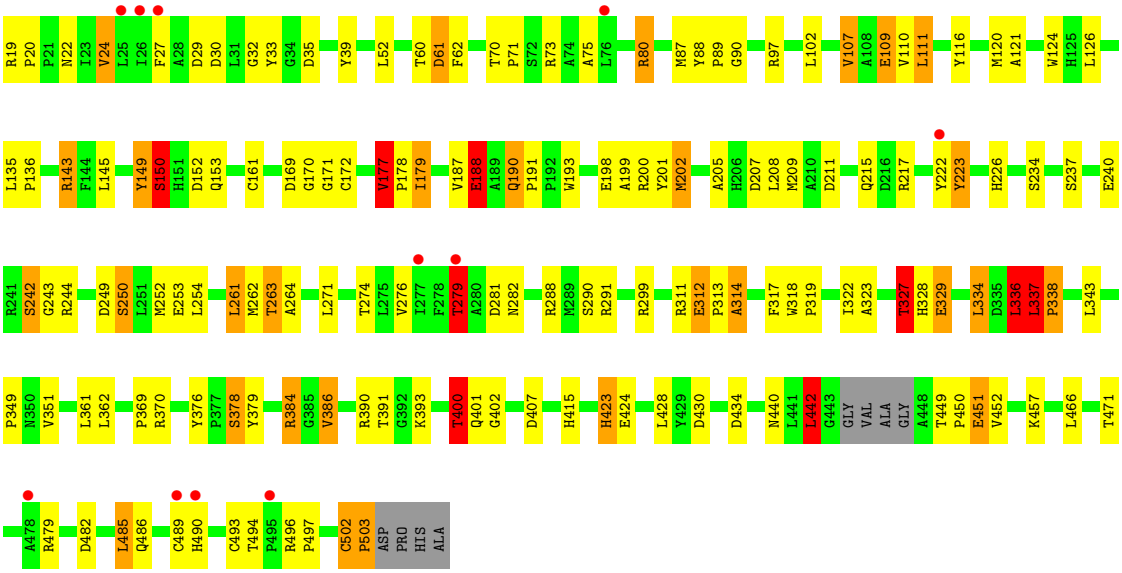
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	P	171	171	171	0	0

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: 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	131.75Å 131.75Å 192.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 28.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.40) 99.3 (28.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.243 0.167 , 0.218	Depositor DCC
R_{free} test set	1628 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 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	0.96	EDS
Total number of atoms	3740	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: NAG, 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	0.96	2/3647 (0.1%)	1.99	109/4987 (2.2%)

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	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	503	PRO	N-CD	6.55	1.57	1.47
1	P	243	GLY	N-CA	5.15	1.53	1.46

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	291	ARG	CD-NE-CZ	23.18	156.05	123.60
1	P	390	ARG	NE-CZ-NH1	21.52	131.06	120.30
1	P	390	ARG	NE-CZ-NH2	-15.40	112.60	120.30
1	P	291	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	P	109	GLU	OE1-CD-OE2	-11.65	109.32	123.30
1	P	281	ASP	CB-CG-OD1	11.50	128.65	118.30
1	P	244	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	P	73	ARG	CD-NE-CZ	11.16	139.23	123.60
1	P	143	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	P	80	ARG	NE-CZ-NH2	10.74	125.67	120.30
1	P	179	ILE	CA-CB-CG2	10.55	132.00	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	479	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	P	336	LEU	CB-CA-C	10.16	129.51	110.20
1	P	299	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	P	35	ASP	CB-CG-OD2	-9.54	109.72	118.30
1	P	33	TYR	CB-CG-CD1	-9.19	115.49	121.00
1	P	52	LEU	CA-CB-CG	8.82	135.59	115.30
1	P	29	ASP	CB-CG-OD2	8.77	126.20	118.30
1	P	207	ASP	CB-CG-OD2	-8.76	110.41	118.30
1	P	384	ARG	CD-NE-CZ	-8.70	111.42	123.60
1	P	143	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	P	479	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	P	244	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	P	329	GLU	OE1-CD-OE2	7.83	132.69	123.30
1	P	169	ASP	CB-CG-OD1	-7.81	111.27	118.30
1	P	242	SER	C-N-CA	-7.79	105.94	122.30
1	P	291	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	P	337	LEU	CA-CB-CG	7.39	132.29	115.30
1	P	489	CYS	CA-CB-SG	-7.15	101.12	114.00
1	P	279	THR	CA-CB-OG1	7.11	123.94	109.00
1	P	288	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	P	250	SER	CB-CA-C	7.00	123.40	110.10
1	P	217	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	P	249	ASP	CB-CG-OD1	6.93	124.54	118.30
1	P	39	TYR	CG-CD1-CE1	-6.93	115.75	121.30
1	P	39	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	P	222	TYR	CB-CG-CD1	6.79	125.07	121.00
1	P	281	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	P	61	ASP	CB-CG-OD1	6.77	124.40	118.30
1	P	170	GLY	CA-C-N	6.76	129.73	116.20
1	P	73	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	P	107	VAL	CB-CA-C	-6.71	98.65	111.40
1	P	80	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	P	311	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	P	234	SER	N-CA-CB	6.65	120.47	110.50
1	P	386	VAL	CG1-CB-CG2	-6.58	100.38	110.90
1	P	116	TYR	CB-CG-CD1	6.57	124.94	121.00
1	P	312	GLU	CG-CD-OE1	6.55	131.39	118.30
1	P	434	ASP	CB-CG-OD1	6.52	124.17	118.30
1	P	370	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	P	424	GLU	CA-C-O	-6.45	106.56	120.10
1	P	188	GLU	OE1-CD-OE2	6.44	131.03	123.30
1	P	87	MET	CG-SD-CE	-6.42	89.93	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	496	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	P	494	THR	CA-C-O	-6.30	106.87	120.10
1	P	171	GLY	N-CA-C	6.28	128.81	113.10
1	P	378	SER	CB-CA-C	-6.24	98.25	110.10
1	P	177	VAL	N-CA-CB	-6.24	97.78	111.50
1	P	327	THR	CB-CA-C	-6.21	94.82	111.60
1	P	311	ARG	CD-NE-CZ	6.21	132.29	123.60
1	P	442	LEU	O-C-N	-6.16	112.73	123.20
1	P	299	ARG	N-CA-CB	-6.13	99.57	110.60
1	P	97	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	P	170	GLY	CA-C-O	-6.12	109.59	120.60
1	P	327	THR	C-N-CA	6.05	136.82	121.70
1	P	323	ALA	N-CA-CB	-6.01	101.69	110.10
1	P	120	MET	CG-SD-CE	-6.00	90.59	100.20
1	P	327	THR	CA-CB-CG2	5.99	120.78	112.40
1	P	494	THR	O-C-N	5.95	132.41	121.10
1	P	29	ASP	OD1-CG-OD2	-5.95	112.00	123.30
1	P	424	GLU	O-C-N	5.90	132.32	121.10
1	P	401	GLN	N-CA-CB	-5.89	100.00	110.60
1	P	299	ARG	NH1-CZ-NH2	5.87	125.86	119.40
1	P	193	TRP	CB-CG-CD1	5.83	134.58	127.00
1	P	177	VAL	CA-CB-CG1	5.82	119.63	110.90
1	P	496	ARG	CA-C-O	-5.81	107.90	120.10
1	P	489	CYS	C-N-CA	5.79	136.17	121.70
1	P	250	SER	N-CA-CB	-5.78	101.82	110.50
1	P	262	MET	CA-CB-CG	5.75	123.08	113.30
1	P	279	THR	CB-CA-C	-5.74	96.10	111.60
1	P	279	THR	N-CA-CB	5.69	121.11	110.30
1	P	336	LEU	CA-C-N	5.67	129.69	117.20
1	P	336	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	P	187	VAL	CG1-CB-CG2	5.59	119.85	110.90
1	P	338	PRO	O-C-N	-5.58	113.78	122.70
1	P	430	ASP	CB-CG-OD1	5.55	123.29	118.30
1	P	179	ILE	CB-CG1-CD1	-5.52	98.45	113.90
1	P	386	VAL	CA-CB-CG1	-5.50	102.66	110.90
1	P	190	GLN	CG-CD-NE2	5.46	129.80	116.70
1	P	271	LEU	N-CA-CB	5.45	121.29	110.40
1	P	170	GLY	C-N-CA	-5.40	110.96	122.30
1	P	30	ASP	CB-CG-OD1	5.38	123.14	118.30
1	P	253	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	P	193	TRP	CB-CG-CD2	-5.36	119.64	126.60
1	P	242	SER	CA-C-N	5.36	126.91	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	312	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	P	391	THR	OG1-CB-CG2	-5.33	97.75	110.00
1	P	423	HIS	CA-CB-CG	-5.33	104.55	113.60
1	P	497	PRO	CA-N-CD	-5.31	104.06	111.50
1	P	400	THR	N-CA-CB	-5.31	100.22	110.30
1	P	150	SER	N-CA-CB	5.26	118.39	110.50
1	P	314	ALA	CB-CA-C	5.22	117.94	110.10
1	P	393	LYS	N-CA-CB	-5.18	101.28	110.60
1	P	143	ARG	CD-NE-CZ	5.15	130.81	123.60
1	P	244	ARG	O-C-N	-5.15	114.45	123.20
1	P	502	CYS	C-N-CD	5.15	139.21	128.40
1	P	39	TYR	CZ-CE2-CD2	-5.14	115.17	119.80
1	P	202	MET	CG-SD-CE	5.14	108.42	100.20
1	P	223	TYR	CB-CG-CD2	5.07	124.04	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	150	SER	Mainchain
1	P	223	TYR	Mainchain
1	P	263	THR	Mainchain
1	P	32	GLY	Mainchain
1	P	327	THR	Mainchain
1	P	336	LEU	Mainchain
1	P	442	LEU	Mainchain
1	P	90	GLY	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	3540	0	3400	70	1
2	A	28	0	25	1	0
3	P	1	0	0	0	0
4	P	171	0	0	11	0
All	All	3740	0	3425	70	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 10.

All (70) 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:102:LEU:O	4:P:2039:HOH:O	1.72	1.06
1:P:109:GLU:OE1	4:P:2043:HOH:O	1.77	1.01
1:P:198:GLU:HG3	4:P:2077:HOH:O	1.61	0.98
1:P:386:VAL:HG11	1:P:466:LEU:HD23	1.55	0.88
1:P:423:HIS:HD2	4:P:2149:HOH:O	1.58	0.84
1:P:109:GLU:OE2	4:P:2043:HOH:O	2.00	0.79
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.71	0.73
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.22	0.69
1:P:135:LEU:HB3	1:P:136:PRO:HD2	1.79	0.65
1:P:376:TYR:CZ	1:P:386:VAL:HG12	2.31	0.64
1:P:242:SER:N	1:P:252:MET:HE1	2.13	0.64
1:P:327:THR:HG23	4:P:2114:HOH:O	1.97	0.64
1:P:150:SER:H	1:P:153:GLN:HE21	1.47	0.62
1:P:400:THR:HG23	4:P:2147:HOH:O	2.00	0.62
1:P:198:GLU:CG	4:P:2077:HOH:O	2.31	0.61
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.82	0.60
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.85	0.59
1:P:19:ARG:N	1:P:20:PRO:HD2	2.20	0.56
1:P:312:GLU:HB3	1:P:313:PRO:HD2	1.87	0.56
1:P:188:GLU:HG3	1:P:188:GLU:O	2.08	0.54
1:P:202:MET:SD	1:P:261:LEU:HD13	2.48	0.53
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.92	0.53
1:P:152:ASP:O	1:P:172:CYS:HB3	2.10	0.52
1:P:428:LEU:H	1:P:440:ASN:ND2	2.08	0.52
1:P:24:VAL:HG11	1:P:276:VAL:HG22	1.91	0.52
1:P:400:THR:CG2	4:P:2147:HOH:O	2.56	0.51
1:P:327:THR:HG21	1:P:361:LEU:HD11	1.92	0.51
1:P:24:VAL:HG13	1:P:276:VAL:HG22	1.94	0.50
1:P:263:THR:O	1:P:264:ALA:C	2.48	0.50
1:P:327:THR:HG22	1:P:329:GLU:H	1.75	0.50
1:P:22:ASN:HB2	1:P:274:THR:OG1	2.12	0.50
1:P:211:ASP:O	1:P:215:GLN:HG3	2.12	0.50
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.14	0.48
1:P:407:ASP:CB	4:P:2143:HOH:O	2.62	0.48
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.49	0.47
1:P:150:SER:H	1:P:153:GLN:NE2	2.11	0.47
1:P:318:TRP:CB	1:P:322:ILE:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:24:VAL:HG13	1:P:276:VAL:HA	1.97	0.47
1:P:317:PHE:CZ	1:P:319:PRO:HG3	2.51	0.46
1:P:205:ALA:O	1:P:209:MET:HG3	2.16	0.46
1:P:502:CYS:SG	1:P:502:CYS:O	2.74	0.46
1:P:415:HIS:CD2	4:P:2146:HOH:O	2.69	0.46
1:P:80:ARG:HG2	1:P:80:ARG:HH11	1.82	0.45
1:P:149:TYR:HB2	1:P:153:GLN:NE2	2.32	0.45
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.52	0.44
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.30	0.44
1:P:199:ALA:O	1:P:200:ARG:C	2.56	0.44
1:P:80:ARG:HG2	1:P:80:ARG:NH1	2.32	0.44
1:P:110:VAL:HG12	1:P:111:LEU:HD13	2.00	0.44
1:P:336:LEU:C	1:P:336:LEU:HD23	2.37	0.44
1:P:70:THR:N	1:P:71:PRO:HD2	2.33	0.43
1:P:279:THR:CG2	1:P:313:PRO:O	2.66	0.43
1:P:279:THR:HG23	1:P:313:PRO:O	2.19	0.42
1:P:400:THR:HB	1:P:423:HIS:CE1	2.54	0.42
1:P:143:ARG:HB3	2:A:1:NAG:H82	2.02	0.42
1:P:449:THR:HG22	1:P:452:VAL:H	1.83	0.42
1:P:88:TYR:HB2	1:P:89:PRO:HA	2.01	0.42
1:P:384:ARG:HH11	1:P:384:ARG:HD3	1.50	0.42
1:P:121:ALA:HA	1:P:145:LEU:O	2.20	0.42
1:P:449:THR:HA	1:P:450:PRO:HD3	1.90	0.41
1:P:402:GLY:HA3	1:P:415:HIS:O	2.20	0.41
1:P:482:ASP:HB3	1:P:485:LEU:HD22	2.02	0.41
1:P:337:LEU:HD12	1:P:338:PRO:N	2.35	0.41
1:P:386:VAL:CG1	1:P:466:LEU:HD23	2.37	0.41
1:P:190:GLN:HA	1:P:191:PRO:HA	1.74	0.41
1:P:150:SER:N	1:P:153:GLN:HE21	2.18	0.40
1:P:449:THR:HG22	1:P:451:GLU:H	1.86	0.40
1:P:378:SER:HB2	1:P:379:TYR:HD1	1.86	0.40
1:P:485:LEU:HD12	1:P:485:LEU:HA	1.89	0.40
1:P:177:VAL:HA	1:P:178:PRO:HD3	2.01	0.40

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]	2.16	0.04

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%)	455 (95%)	21 (4%)	1 (0%)	47 62

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	367/385 (95%)	332 (90%)	35 (10%)	8 12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	VAL
1	P	27	PHE
1	P	61	ASP
1	P	107	VAL
1	P	111	LEU
1	P	149	TYR
1	P	161	CYS
1	P	177	VAL
1	P	179	ILE
1	P	188	GLU

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Mol	Chain	Res	Type
1	P	208	LEU
1	P	237	SER
1	P	240	GLU
1	P	250	SER
1	P	254	LEU
1	P	261	LEU
1	P	279	THR
1	P	282	ASN
1	P	290	SER
1	P	327	THR
1	P	334	LEU
1	P	336	LEU
1	P	337	LEU
1	P	343	LEU
1	P	349	PRO
1	P	351	VAL
1	P	362	LEU
1	P	369	PRO
1	P	400	THR
1	P	442	LEU
1	P	451	GLU
1	P	457	LYS
1	P	471	THR
1	P	485	LEU
1	P	503	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	153	GLN
1	P	226	HIS
1	P	328	HIS
1	P	423	HIS
1	P	440	ASN
1	P	465	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	1,2	14,14,15	1.81	5 (35%)	17,19,21	3.36	11 (64%)
2	NAG	A	2	2	14,14,15	1.28	2 (14%)	17,19,21	2.19	6 (35%)

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	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	A	2	2	1/1/5/7	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O7-C7	-3.38	1.15	1.23
2	A	1	NAG	C2-N2	2.90	1.51	1.46
2	A	2	NAG	O7-C7	-2.89	1.16	1.23
2	A	1	NAG	O4-C4	-2.88	1.36	1.43
2	A	1	NAG	O5-C5	-2.88	1.37	1.43
2	A	2	NAG	C2-N2	2.44	1.50	1.46
2	A	1	NAG	C4-C5	2.08	1.57	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	NAG	C1-O5-C5	5.37	119.47	112.19
2	A	1	NAG	O4-C4-C3	5.37	122.76	110.35
2	A	1	NAG	C1-O5-C5	5.26	119.32	112.19
2	A	1	NAG	O7-C7-N2	-5.25	112.30	121.95
2	A	1	NAG	C8-C7-N2	5.10	124.73	116.10
2	A	1	NAG	O5-C1-C2	4.90	119.02	111.29
2	A	1	NAG	O4-C4-C5	-4.03	99.30	109.30
2	A	2	NAG	C2-N2-C7	-3.82	117.46	122.90
2	A	1	NAG	O5-C5-C6	3.72	113.04	107.20
2	A	2	NAG	O3-C3-C2	-3.51	102.21	109.47
2	A	1	NAG	C2-N2-C7	-2.56	119.25	122.90
2	A	2	NAG	C3-C4-C5	2.34	114.42	110.24
2	A	1	NAG	C6-C5-C4	-2.25	107.72	113.00
2	A	1	NAG	O3-C3-C2	2.25	114.12	109.47
2	A	2	NAG	O7-C7-C8	2.21	126.17	122.06
2	A	1	NAG	C3-C4-C5	-2.11	106.48	110.24
2	A	2	NAG	C8-C7-N2	-2.10	112.55	116.10

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	2	NAG	O5-C5-C6-O6
2	A	1	NAG	C1-C2-N2-C7

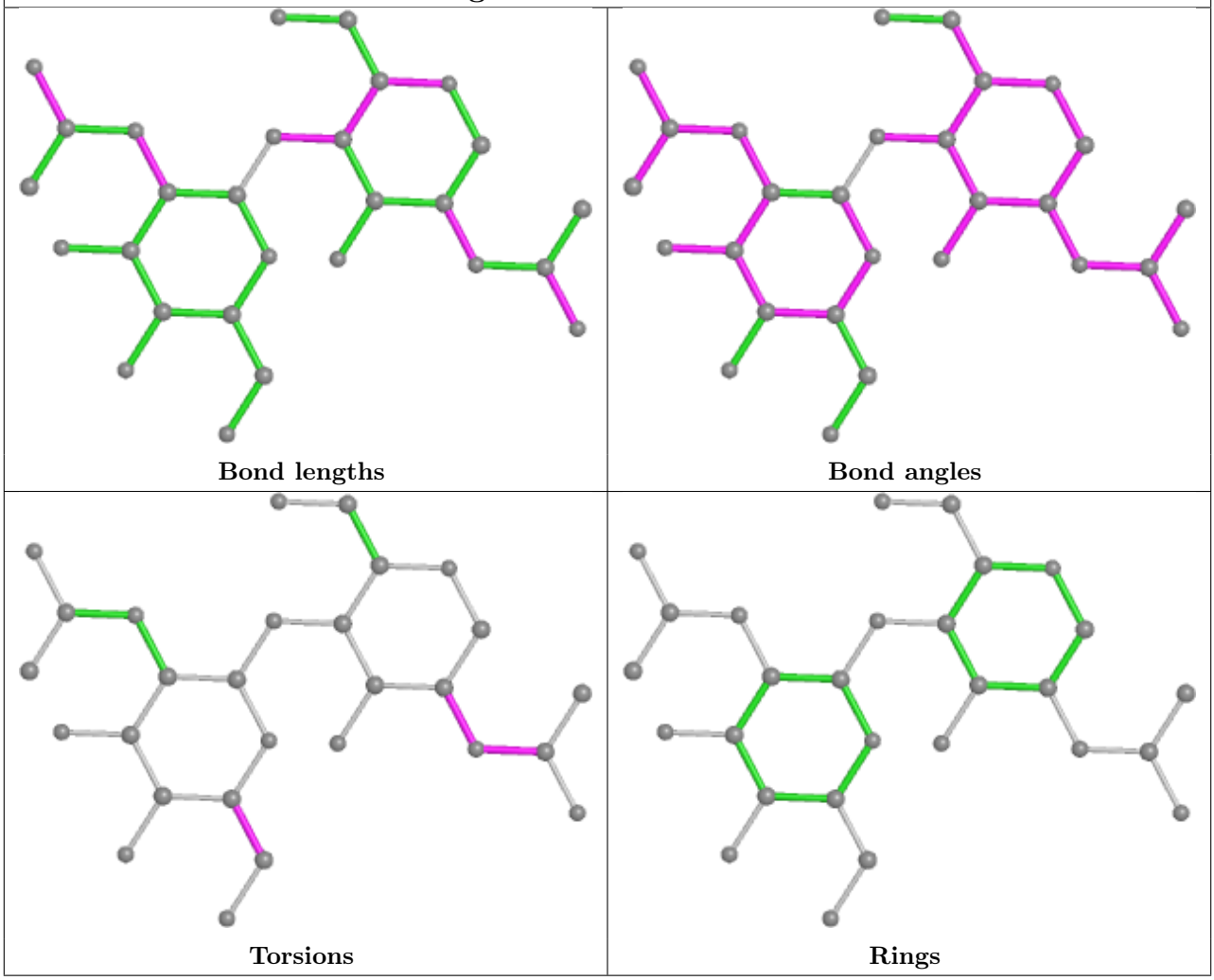
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	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 A



5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 (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	P	481/489 (98%)	-0.26	11 (2%) 60 58	20, 37, 61, 84	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	26	ILE	4.1
1	P	478	ALA	3.9
1	P	25	LEU	3.4
1	P	490	HIS	3.4
1	P	222	TYR	2.9
1	P	279	THR	2.6
1	P	27	PHE	2.5
1	P	495	PRO	2.4
1	P	76	LEU	2.4
1	P	489	CYS	2.3
1	P	277	ILE	2.2

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	NAG	A	2	14/15	0.81	0.25	77,83,94,97	0

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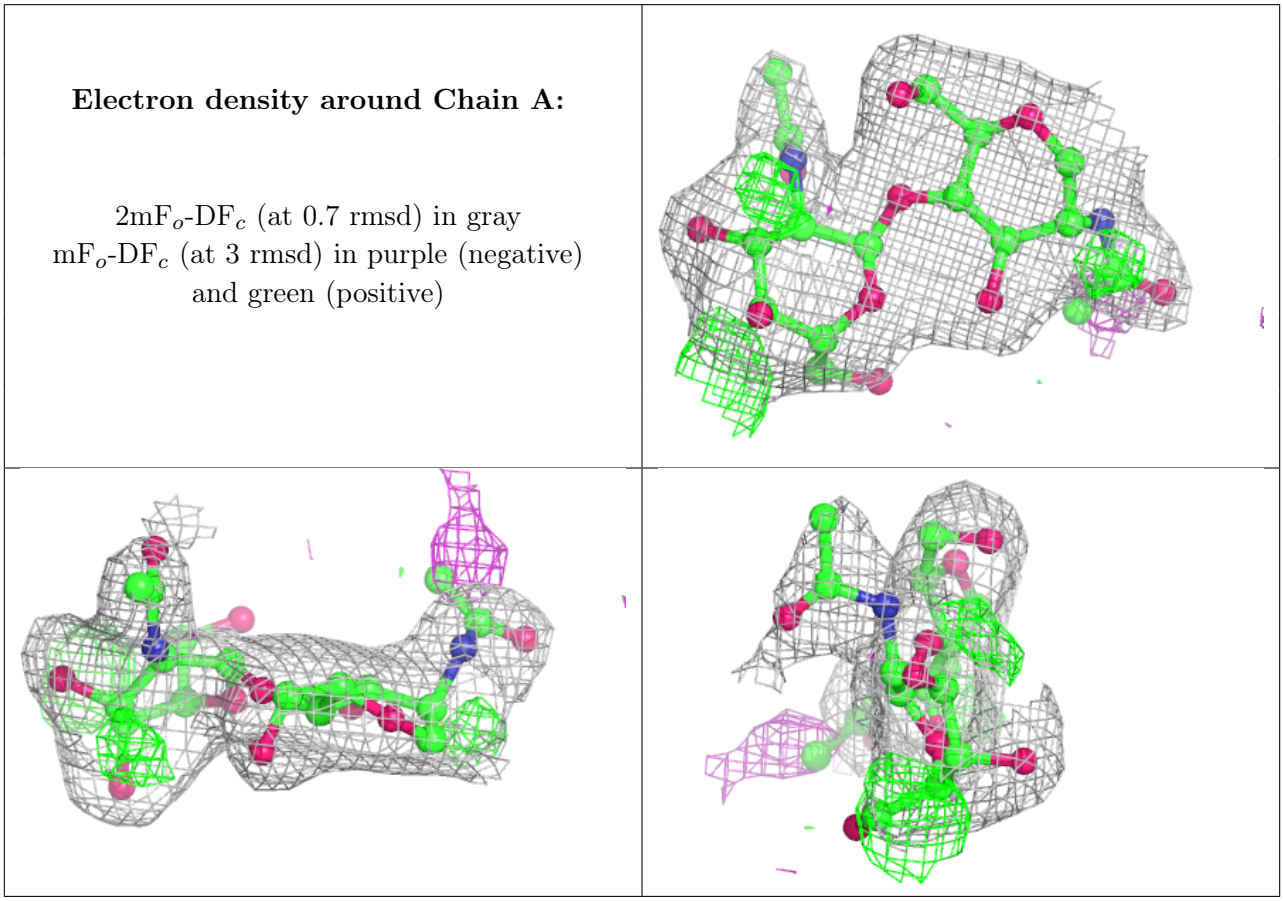
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	1	14/15	0.94	0.17	45,57,70,70	0

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
3	MG	P	700	1/1	0.95	0.12	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.