



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:49 AM UTC

PDB ID : 1E1Z / pdb_00001e1z
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 ⓘ 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

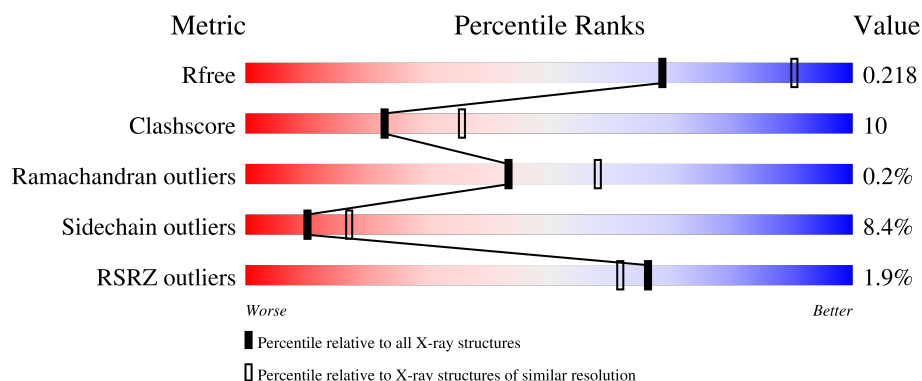
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

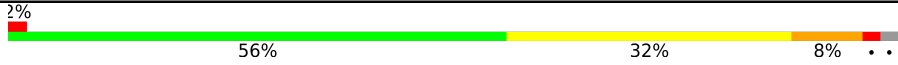
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	P	489	
2	A	2	

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
1	P	481	Total	C	N	O	S	0	0	0
			3540	2263	599	655	23			

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
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

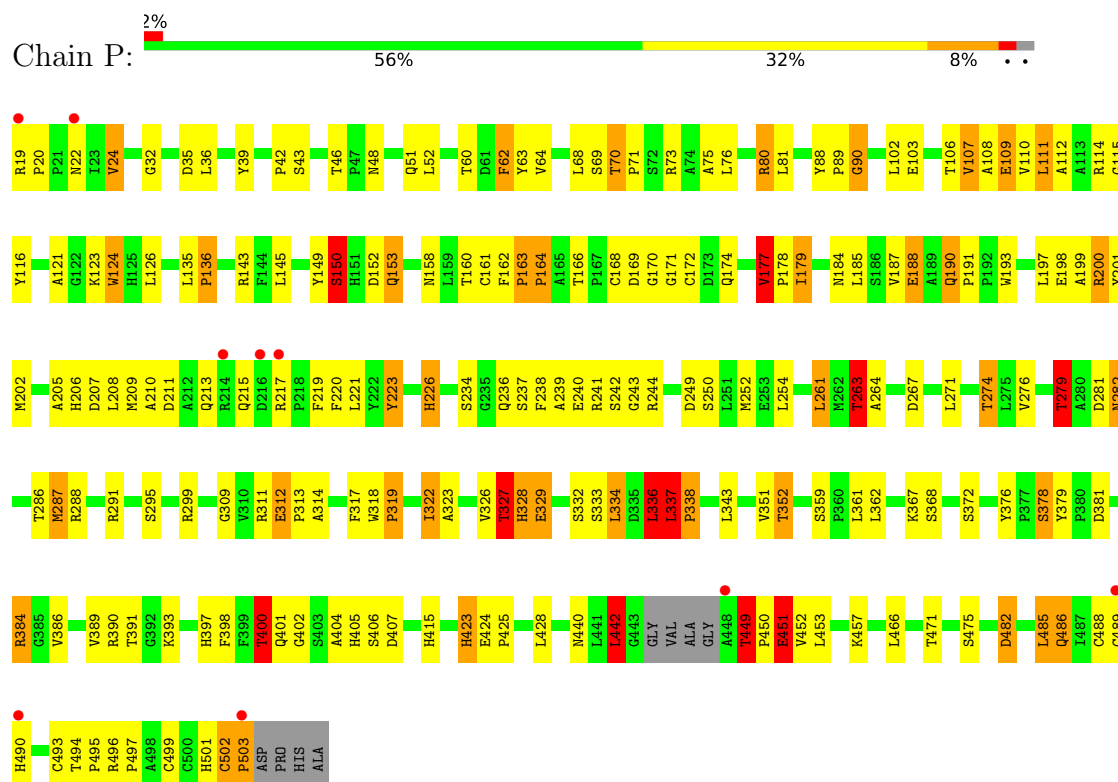
- Molecule 4 is water.

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

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: Arylsulfatase A



• Molecule 2: 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	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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.40) 99.2 (30.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.90%)	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)	0.35 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

5.1 Standard geometry

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

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	1.25	8/3647 (0.2%)	2.39	213/4987 (4.3%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	327	THR	CA-C	6.96	1.60	1.52
1	P	503	PRO	N-CD	6.62	1.57	1.47
1	P	243	GLY	N-CA	5.80	1.53	1.45
1	P	359	SER	N-CA	5.66	1.52	1.46
1	P	502	CYS	C-O	-5.49	1.17	1.24
1	P	70	THR	N-CA	-5.36	1.42	1.46
1	P	73	ARG	NE-CZ	-5.19	1.27	1.33
1	P	328	HIS	CD2-NE2	5.03	1.43	1.37

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	291	ARG	CD-NE-CZ	22.61	156.05	124.40
1	P	494	THR	O-C-N	15.08	132.41	121.85
1	P	494	THR	CA-C-O	-12.78	106.87	119.91
1	P	179	ILE	CA-CB-CG2	12.65	132.00	110.50
1	P	496	ARG	CA-C-O	-12.09	107.90	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	73	ARG	CD-NE-CZ	10.59	139.23	124.40
1	P	190	GLN	OE1-CD-NE2	-10.59	112.01	122.60
1	P	236	GLN	OE1-CD-NE2	10.07	132.67	122.60
1	P	171	GLY	N-CA-C	10.03	128.81	114.67
1	P	107	VAL	CB-CA-C	-10.00	98.65	112.14
1	P	424	GLU	CA-C-O	-9.93	106.56	120.16
1	P	166	THR	CA-C-O	9.60	128.56	119.24
1	P	177	VAL	N-CA-CB	-9.59	97.78	111.21
1	P	424	GLU	O-C-N	9.56	132.32	121.32
1	P	390	ARG	NE-CZ-NH1	9.56	131.06	121.50
1	P	279	THR	CA-CB-OG1	9.56	123.94	109.60
1	P	489	CYS	CA-C-N	9.41	136.17	123.46
1	P	489	CYS	C-N-CA	9.41	136.17	123.46
1	P	336	LEU	CB-CA-C	9.34	129.51	109.99
1	P	384	ARG	CD-NE-CZ	-9.27	111.42	124.40
1	P	423	HIS	CA-CB-CG	-9.26	104.55	113.80
1	P	327	THR	CA-C-N	9.24	136.82	122.49
1	P	327	THR	C-N-CA	9.24	136.82	122.49
1	P	190	GLN	CG-CD-NE2	8.94	129.80	116.40
1	P	35	ASP	CA-C-O	-8.61	109.63	119.79
1	P	179	ILE	N-CA-CB	-8.55	102.12	110.08
1	P	279	THR	CB-CA-C	-8.53	96.10	114.10
1	P	327	THR	CB-CA-C	-7.95	94.82	109.37
1	P	153	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	P	242	SER	CA-C-N	-7.89	105.94	121.41
1	P	242	SER	C-N-CA	-7.89	105.94	121.41
1	P	442	LEU	O-C-N	-7.82	112.73	122.35
1	P	197	LEU	CA-C-O	7.77	128.79	120.55
1	P	397	HIS	CA-CB-CG	7.76	121.56	113.80
1	P	174	GLN	CG-CD-NE2	7.68	127.92	116.40
1	P	271	LEU	N-CA-CB	7.55	121.29	109.82
1	P	352	THR	CA-C-N	7.52	133.83	122.93
1	P	352	THR	C-N-CA	7.52	133.83	122.93
1	P	249	ASP	CA-CB-CG	-7.37	105.23	112.60
1	P	502	CYS	CA-C-O	7.36	130.24	120.16
1	P	170	GLY	CA-C-N	-7.35	110.96	122.86
1	P	170	GLY	C-N-CA	-7.35	110.96	122.86
1	P	390	ARG	NE-CZ-NH2	-7.34	112.60	119.20
1	P	179	ILE	CB-CG1-CD1	-7.31	98.45	113.80
1	P	107	VAL	N-CA-CB	7.21	120.35	110.54
1	P	267	ASP	CA-C-O	-7.20	112.85	120.63
1	P	226	HIS	CA-CB-CG	-7.20	106.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	80	ARG	NE-CZ-NH2	7.19	125.67	119.20
1	P	206	HIS	CA-CB-CG	-7.17	106.63	113.80
1	P	381	ASP	CA-C-O	7.06	128.78	121.23
1	P	90	GLY	O-C-N	-7.05	115.27	122.60
1	P	338	PRO	O-C-N	-6.94	113.78	122.17
1	P	267	ASP	CA-CB-CG	-6.93	105.67	112.60
1	P	174	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	P	238	PHE	CA-CB-CG	-6.82	106.98	113.80
1	P	179	ILE	CB-CA-C	6.76	118.19	110.89
1	P	378	SER	CB-CA-C	-6.69	98.25	110.63
1	P	398	PHE	CA-CB-CG	-6.69	107.11	113.80
1	P	43	SER	N-CA-C	-6.65	106.12	114.56
1	P	190	GLN	CB-CG-CD	6.64	123.89	112.60
1	P	46	THR	O-C-N	-6.63	115.63	121.20
1	P	372	SER	CA-CB-OG	-6.63	97.83	111.10
1	P	250	SER	CB-CA-C	6.63	123.40	110.67
1	P	220	PHE	CA-C-O	-6.61	113.19	120.33
1	P	451	GLU	CB-CG-CD	6.61	123.83	112.60
1	P	299	ARG	N-CA-CB	-6.58	99.57	110.23
1	P	442	LEU	N-CA-CB	-6.55	100.94	110.70
1	P	279	THR	N-CA-CB	6.52	121.11	110.55
1	P	336	LEU	CA-C-O	-6.49	111.27	119.31
1	P	401	GLN	N-CA-CB	-6.49	100.00	110.77
1	P	184	ASN	CA-CB-CG	-6.42	106.17	112.60
1	P	187	VAL	CB-CA-C	-6.42	104.30	111.23
1	P	51	GLN	CB-CG-CD	-6.39	101.73	112.60
1	P	103	GLU	CA-C-O	-6.39	112.62	119.97
1	P	136	PRO	N-CA-C	6.37	118.48	110.70
1	P	486	GLN	CA-C-N	6.36	129.09	120.63
1	P	486	GLN	C-N-CA	6.36	129.09	120.63
1	P	381	ASP	O-C-N	-6.34	116.63	123.42
1	P	112	ALA	N-CA-C	-6.34	104.45	111.36
1	P	114	ARG	CA-C-O	6.34	127.07	119.59
1	P	115	GLY	N-CA-C	6.33	124.69	115.32
1	P	170	GLY	CA-C-O	-6.31	109.59	120.57
1	P	242	SER	CA-C-O	-6.30	114.22	121.47
1	P	488	CYS	CA-C-N	6.27	129.53	120.38
1	P	488	CYS	C-N-CA	6.27	129.53	120.38
1	P	123	LYS	CA-C-O	-6.24	113.58	120.69
1	P	475	SER	CA-C-N	6.24	129.15	120.29
1	P	475	SER	C-N-CA	6.24	129.15	120.29
1	P	184	ASN	OD1-CG-ND2	6.23	128.83	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	323	ALA	N-CA-CB	-6.19	101.69	110.04
1	P	263	THR	O-C-N	-6.18	115.42	122.09
1	P	333	SER	O-C-N	-6.16	115.02	122.22
1	P	299	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	P	401	GLN	N-CA-C	6.14	117.73	108.46
1	P	404	ALA	CA-C-O	-6.13	112.92	119.97
1	P	400	THR	N-CA-CB	-6.08	100.22	111.53
1	P	106	THR	CA-C-O	-6.07	114.79	121.89
1	P	327	THR	OG1-CB-CG2	6.07	121.43	109.30
1	P	327	THR	CA-CB-CG2	6.05	120.78	110.50
1	P	46	THR	CA-C-N	6.04	125.75	119.05
1	P	46	THR	C-N-CA	6.04	125.75	119.05
1	P	239	ALA	CA-C-O	-6.02	113.78	120.70
1	P	322	ILE	CA-C-O	-6.00	114.10	120.53
1	P	405	HIS	CA-CB-CG	-6.00	107.80	113.80
1	P	393	LYS	N-CA-CB	-5.99	101.28	110.44
1	P	63	TYR	N-CA-C	5.97	118.78	109.52
1	P	242	SER	N-CA-C	-5.96	101.65	110.48
1	P	200	ARG	N-CA-C	-5.96	104.69	111.07
1	P	309	GLY	CA-C-N	-5.92	115.57	122.14
1	P	309	GLY	C-N-CA	-5.92	115.57	122.14
1	P	482	ASP	CA-C-N	5.92	125.59	119.56
1	P	482	ASP	C-N-CA	5.92	125.59	119.56
1	P	389	VAL	CA-C-O	-5.90	114.00	120.43
1	P	162	PHE	CA-C-N	5.86	123.88	119.66
1	P	162	PHE	C-N-CA	5.86	123.88	119.66
1	P	326	VAL	CA-C-O	-5.86	114.35	120.27
1	P	425	PRO	N-CA-CB	5.84	109.03	102.60
1	P	207	ASP	CB-CA-C	-5.84	101.09	110.79
1	P	108	ALA	CA-C-N	5.83	128.09	120.28
1	P	108	ALA	C-N-CA	5.83	128.09	120.28
1	P	291	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	P	221	LEU	CA-C-N	5.81	131.74	123.14
1	P	221	LEU	C-N-CA	5.81	131.74	123.14
1	P	244	ARG	O-C-N	-5.78	114.45	122.19
1	P	391	THR	OG1-CB-CG2	-5.78	97.75	109.30
1	P	489	CYS	CA-CB-SG	-5.77	101.12	114.40
1	P	281	ASP	CA-CB-CG	5.77	118.37	112.60
1	P	213	GLN	CA-C-N	5.76	128.00	120.28
1	P	213	GLN	C-N-CA	5.76	128.00	120.28
1	P	114	ARG	N-CA-C	-5.74	105.47	112.88
1	P	164	PRO	CA-C-N	-5.72	111.69	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	164	PRO	C-N-CA	-5.72	111.69	121.08
1	P	337	LEU	CA-C-O	5.68	124.47	119.08
1	P	81	LEU	N-CA-C	-5.67	102.43	109.64
1	P	333	SER	CA-C-O	5.66	126.50	120.10
1	P	109	GLU	OE1-CD-OE2	-5.66	109.32	122.90
1	P	312	GLU	CG-CD-OE1	5.65	131.39	118.40
1	P	223	TYR	O-C-N	-5.65	115.74	122.63
1	P	311	ARG	CD-NE-CZ	5.64	132.29	124.40
1	P	150	SER	N-CA-CB	5.62	118.39	110.36
1	P	51	GLN	CA-C-O	-5.61	114.02	120.24
1	P	36	LEU	CA-C-O	-5.57	115.24	121.81
1	P	495	PRO	N-CD-CG	5.57	110.48	103.80
1	P	168	CYS	O-C-N	-5.56	116.19	122.97
1	P	295	SER	N-CA-C	-5.54	106.10	112.92
1	P	274	THR	N-CA-C	5.54	117.44	108.41
1	P	116	TYR	O-C-N	-5.53	116.49	123.01
1	P	39	TYR	N-CA-C	-5.53	105.75	112.88
1	P	52	LEU	CA-CB-CG	5.51	135.59	116.30
1	P	391	THR	N-CA-CB	5.50	119.41	110.77
1	P	160	THR	CA-CB-OG1	-5.49	101.36	109.60
1	P	70	THR	CA-CB-OG1	-5.49	101.37	109.60
1	P	73	ARG	CA-C-O	-5.48	114.74	120.55
1	P	185	LEU	CA-C-N	-5.46	114.07	122.87
1	P	185	LEU	C-N-CA	-5.46	114.07	122.87
1	P	244	ARG	N-CA-CB	-5.46	103.63	111.54
1	P	250	SER	N-CA-CB	-5.46	101.82	110.28
1	P	281	ASP	N-CA-C	5.43	118.12	111.82
1	P	63	TYR	N-CA-CB	-5.43	102.10	111.55
1	P	177	VAL	CA-CB-CG1	5.43	119.63	110.40
1	P	451	GLU	N-CA-C	-5.43	105.44	111.36
1	P	453	LEU	N-CA-CB	-5.42	101.87	110.22
1	P	158	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	P	64	VAL	O-C-N	-5.41	114.93	121.10
1	P	291	ARG	CA-CB-CG	-5.39	103.31	114.10
1	P	329	GLU	CA-CB-CG	-5.39	103.31	114.10
1	P	226	HIS	N-CA-C	-5.39	106.55	113.23
1	P	287	MET	CA-C-O	-5.36	114.20	120.20
1	P	51	GLN	N-CA-CB	5.35	118.17	110.20
1	P	328	HIS	N-CA-C	-5.34	106.14	113.30
1	P	62	PHE	O-C-N	-5.34	116.43	123.21
1	P	312	GLU	CB-CG-CD	-5.33	103.53	112.60
1	P	68	LEU	CA-C-N	5.31	127.67	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	68	LEU	C-N-CA	5.31	127.67	120.65
1	P	499	CYS	N-CA-C	-5.31	106.06	112.54
1	P	393	LYS	CA-C-O	-5.31	112.85	119.28
1	P	497	PRO	CA-N-CD	-5.31	104.06	111.50
1	P	449	THR	CA-CB-OG1	-5.30	101.65	109.60
1	P	219	PHE	CA-C-N	5.30	130.38	122.86
1	P	219	PHE	C-N-CA	5.30	130.38	122.86
1	P	424	GLU	CB-CG-CD	-5.30	103.60	112.60
1	P	163	PRO	O-C-N	5.29	123.64	121.15
1	P	234	SER	N-CA-CB	5.28	120.47	111.66
1	P	336	LEU	N-CA-CB	-5.27	101.80	110.40
1	P	274	THR	CA-CB-OG1	-5.27	101.69	109.60
1	P	406	SER	CA-C-O	-5.26	113.40	119.56
1	P	286	THR	CA-C-O	5.26	125.85	119.38
1	P	169	ASP	N-CA-CB	5.25	118.96	110.41
1	P	48	ASN	CA-CB-CG	-5.23	107.37	112.60
1	P	368	SER	CA-C-O	5.22	125.89	120.25
1	P	213	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	P	332	SER	O-C-N	-5.14	116.47	123.15
1	P	76	LEU	CA-C-O	-5.13	115.11	120.55
1	P	221	LEU	O-C-N	-5.13	117.23	123.29
1	P	288	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	P	193	TRP	CB-CG-CD1	5.12	134.58	126.90
1	P	319	PRO	CA-C-O	5.12	126.90	121.32
1	P	193	TRP	CB-CG-CD2	-5.12	119.64	126.80
1	P	42	PRO	CA-C-N	-5.10	114.27	122.08
1	P	42	PRO	C-N-CA	-5.10	114.27	122.08
1	P	217	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	P	501	HIS	CA-CB-CG	-5.08	108.72	113.80
1	P	69	SER	N-CA-C	5.08	116.51	110.97
1	P	367	LYS	CA-C-N	-5.07	113.29	120.49
1	P	367	LYS	C-N-CA	-5.07	113.29	120.49
1	P	244	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	P	299	ARG	NH1-CZ-NH2	5.04	125.86	119.30
1	P	359	SER	CA-C-O	5.04	123.23	118.34
1	P	282	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	P	124	TRP	CA-C-N	5.01	129.67	122.40
1	P	124	TRP	C-N-CA	5.01	129.67	122.40
1	P	263	THR	CA-C-O	5.01	125.86	120.70
1	P	423	HIS	O-C-N	-5.01	117.40	123.27

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	3401	73	1
2	A	28	0	25	1	0
3	P	1	0	0	0	0
4	P	171	0	0	12	0
All	All	3740	0	3426	73	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 (73) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:THR:O	1:P:264:ALA:C	2.48	0.55
1:P:241:ARG:CB	1:P:252:MET:HE1	2.37	0.55
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: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:199:ALA:O	1:P:200:ARG:C	2.56	0.49
1:P:336:LEU:C	1:P:336:LEU:HD23	2.37	0.48
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
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:80:ARG:HG2	1:P:80:ARG:NH1	2.32	0.44
1:P:109:GLU:CD	4:P:2043:HOH:O	2.31	0.44
1:P:110:VAL:HG12	1:P:111:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:PRO:HA	1:P:164:PRO:C	2.43	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:210:ALA:O	1:P:211:ASP:C	2.60	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%)	43 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS

5.3.2 Protein sidechains ⓘ

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%)	336 (92%)	31 (8%)	10 17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	VAL
1	P	107	VAL
1	P	111	LEU
1	P	161	CYS
1	P	177	VAL
1	P	179	ILE
1	P	188	GLU
1	P	208	LEU
1	P	237	SER
1	P	240	GLU
1	P	254	LEU
1	P	261	LEU
1	P	279	THR
1	P	282	ASN
1	P	287	MET
1	P	327	THR
1	P	334	LEU
1	P	336	LEU
1	P	337	LEU
1	P	343	LEU

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Mol	Chain	Res	Type
1	P	351	VAL
1	P	352	THR
1	P	362	LEU
1	P	400	THR
1	P	442	LEU
1	P	449	THR
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	138	HIS
1	P	153	GLN
1	P	213	GLN
1	P	226	HIS
1	P	282	ASN
1	P	328	HIS
1	P	423	HIS
1	P	440	ASN
1	P	460	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 ⓘ

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	1.83	5 (35%)	17,19,21	3.35	11 (64%)
2	NAG	A	2	2	14,14,15	1.31	2 (14%)	17,19,21	2.23	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	2,1	1/1/5/7	2/6/23/26	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	-3.42	1.15	1.23
2	A	1	NAG	C2-N2	3.02	1.51	1.46
2	A	1	NAG	O5-C5	-2.98	1.37	1.43
2	A	2	NAG	O7-C7	-2.93	1.16	1.23
2	A	1	NAG	O4-C4	-2.74	1.36	1.43
2	A	2	NAG	C2-N2	2.54	1.50	1.46
2	A	1	NAG	C4-C5	2.06	1.57	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O7-C7-N2	-5.48	112.30	121.98
2	A	2	NAG	C1-O5-C5	5.43	119.47	112.19
2	A	1	NAG	C1-O5-C5	5.32	119.32	112.19
2	A	1	NAG	O4-C4-C3	5.25	122.76	110.38
2	A	1	NAG	C8-C7-N2	5.19	124.73	116.12
2	A	1	NAG	O5-C1-C2	5.00	119.02	111.29
2	A	1	NAG	O4-C4-C5	-4.07	99.30	109.32
2	A	2	NAG	C2-N2-C7	-4.06	117.46	122.90
2	A	2	NAG	O3-C3-C2	-3.46	102.21	109.40
2	A	1	NAG	O5-C5-C6	2.76	113.04	107.66
2	A	1	NAG	C2-N2-C7	-2.72	119.25	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	O7-C7-C8	2.31	126.17	122.05
2	A	2	NAG	C3-C4-C5	2.31	114.42	110.23
2	A	1	NAG	O3-C3-C2	2.27	114.12	109.40
2	A	1	NAG	C6-C5-C4	-2.16	107.72	113.02
2	A	2	NAG	C8-C7-N2	-2.15	112.55	116.12
2	A	1	NAG	C3-C4-C5	-2.07	106.48	110.23

All (2) chirality outliers are listed below:

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

All (3) torsion outliers are listed below:

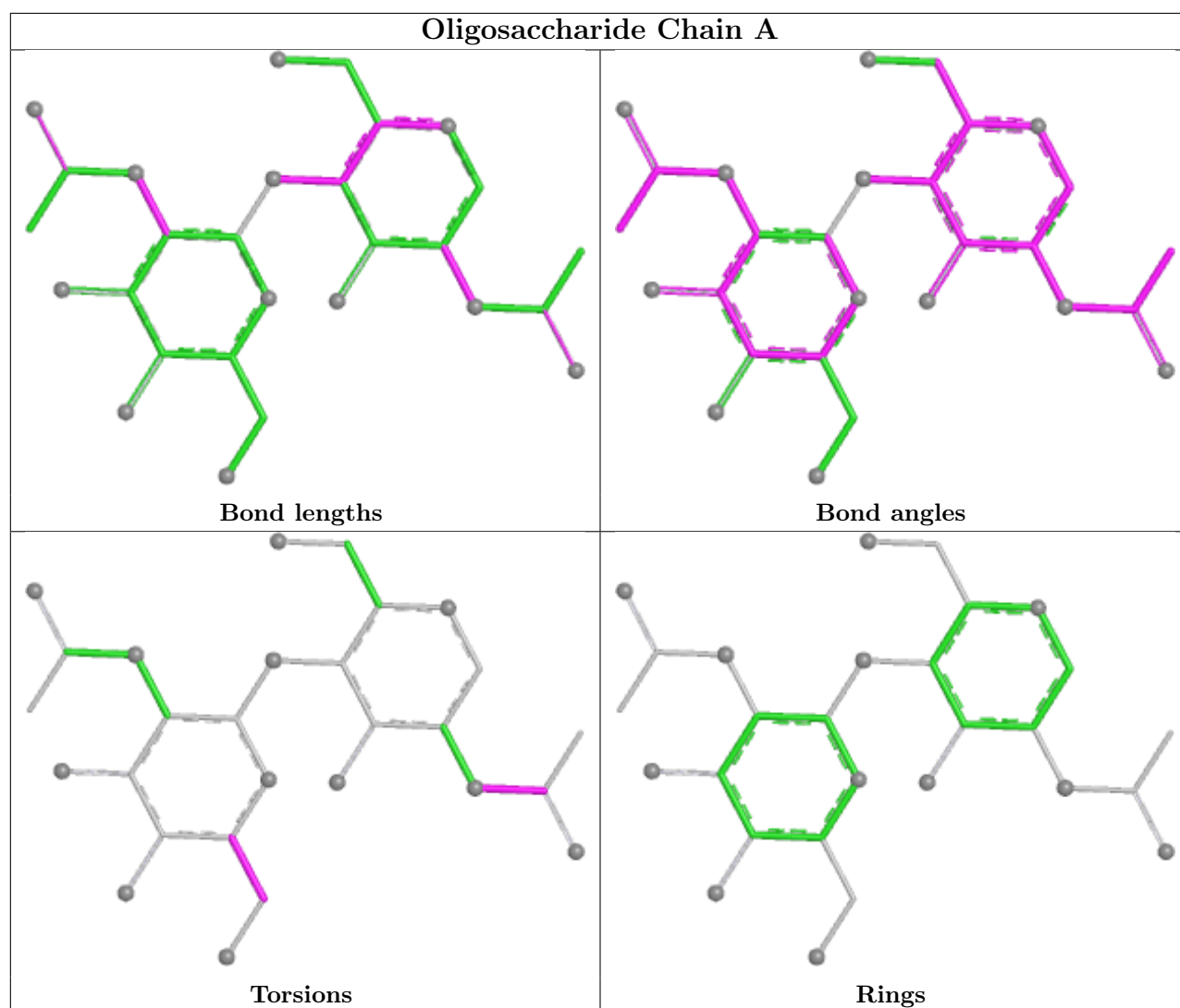
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	A	2	NAG	O5-C5-C6-O6

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.



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 ⓘ

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%)	-0.27	9 (1%) 66 62	20, 37, 61, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	448	ALA	4.7
1	P	490	HIS	4.7
1	P	19	ARG	3.0
1	P	489	CYS	2.9
1	P	216	ASP	2.4
1	P	503	PRO	2.3
1	P	22	ASN	2.1
1	P	214	ARG	2.1
1	P	217	ARG	2.1

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

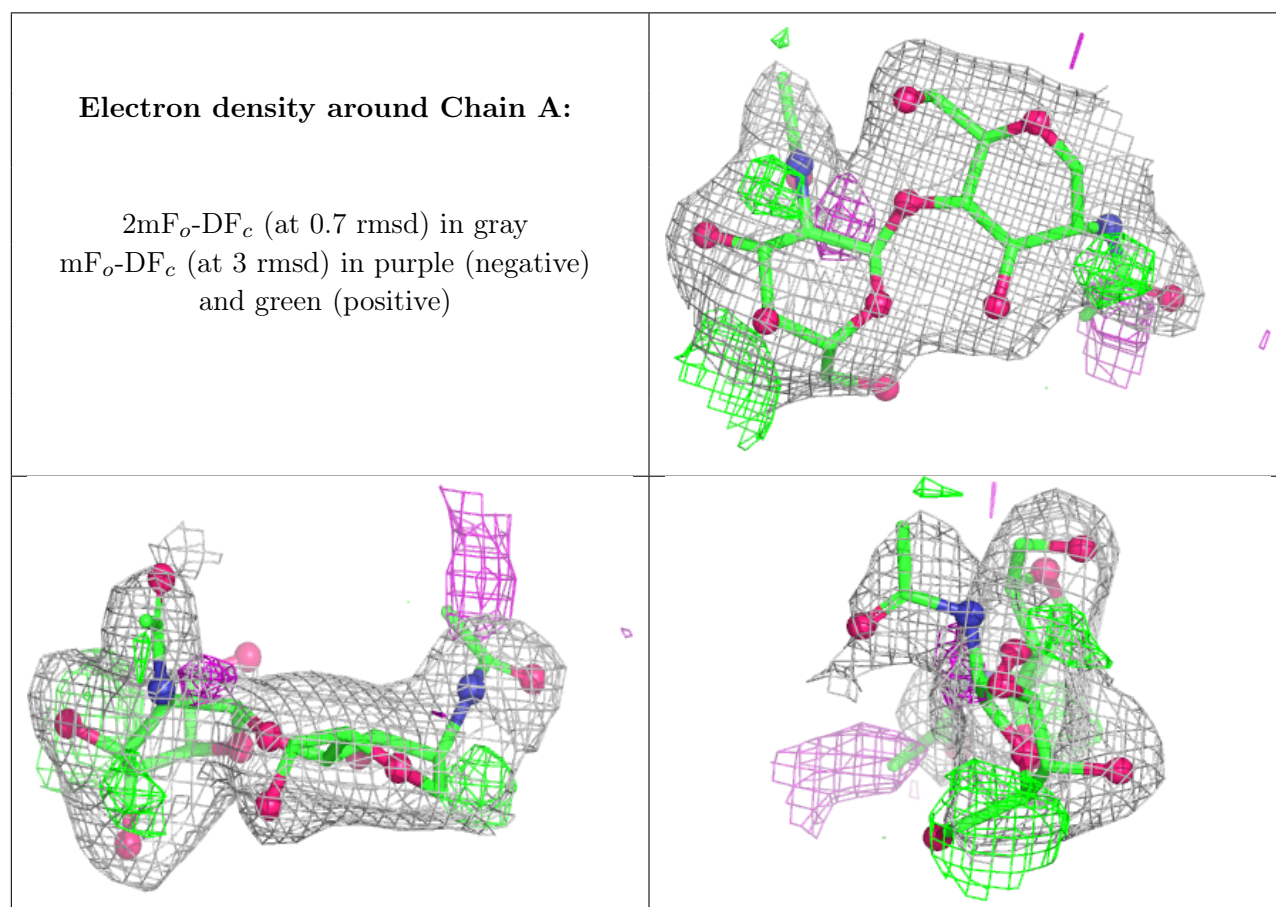
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	A	1	14/15	-	-	45,57,70,70	0
2	NAG	A	2	14/15	-	-	77,83,94,97	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	0.08	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.