



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:02 PM UTC

PDB ID : 1E2S / pdb_00001e2s
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 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

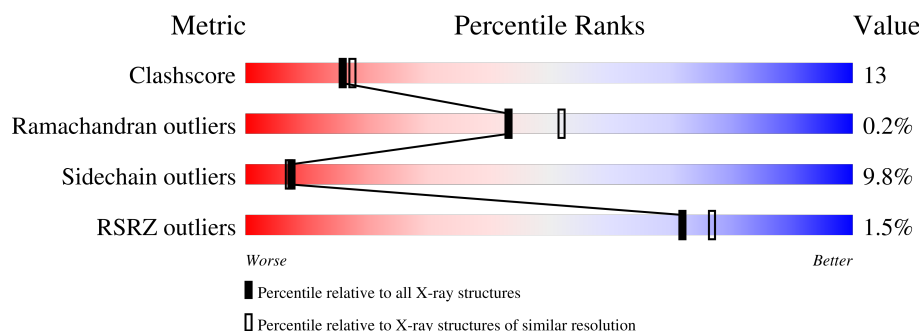
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 $\leq 5\%$. 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	55% 32% 9% ..
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
1	P	481	Total	C	N	O	S	0	0	0
			3553	2270	603	657	23			

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.

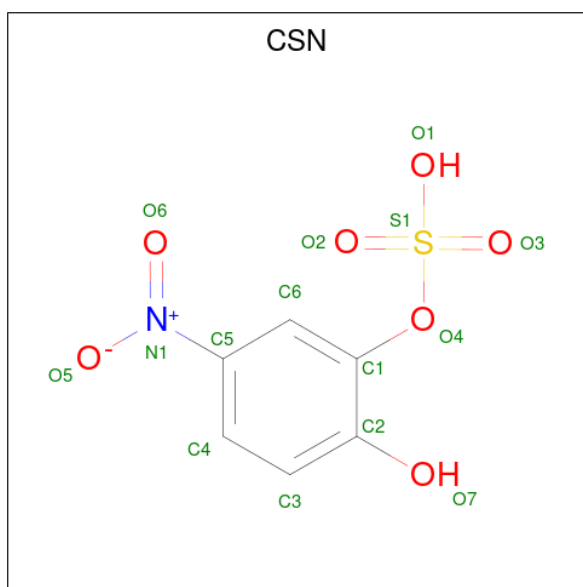


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 N,4-DIHYDROXY-N-OXO-3-(SULFOOXY)BENZENAMINIUM (CCD ID: CSN) (formula: C₆H₅NO₇S).



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

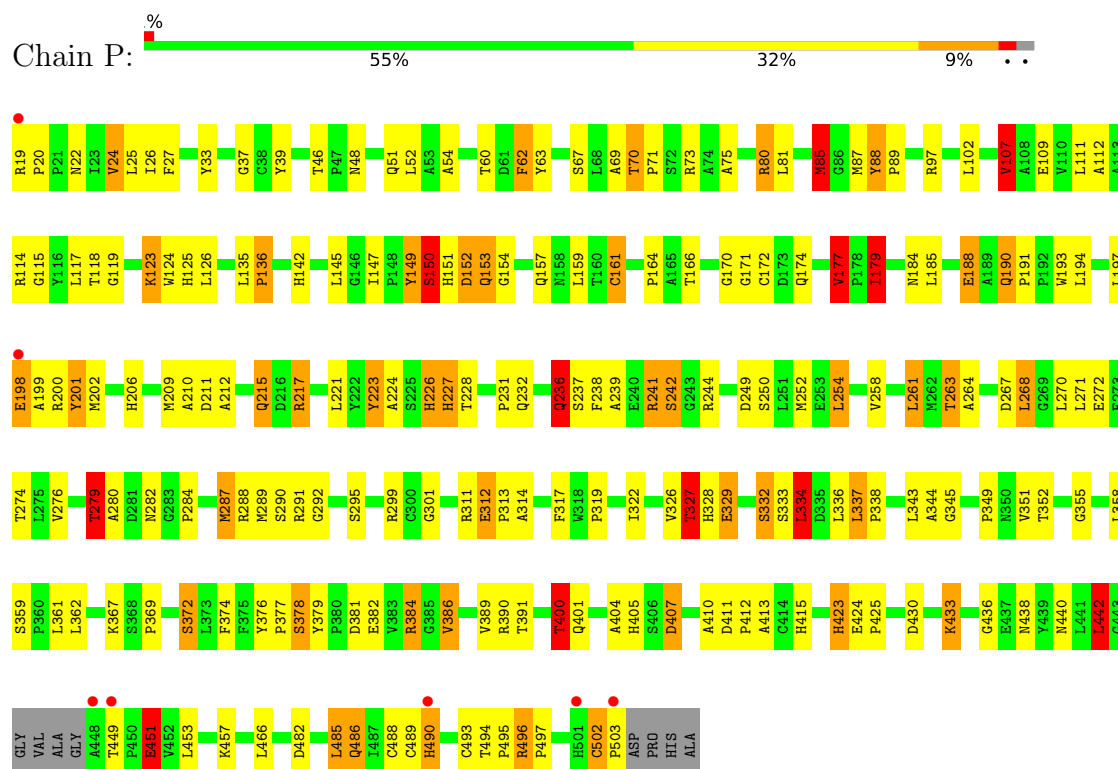
- Molecule 5 is water.

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

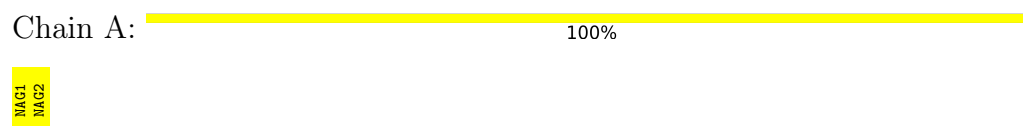
3 Residue-property plots

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	131.80Å 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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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.*

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: CSN, 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	1.21	7/3660 (0.2%)	2.27	193/5003 (3.9%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	149	TYR	C-O	7.88	1.29	1.24
1	P	502	CYS	C-O	-7.38	1.16	1.24
1	P	503	PRO	N-CD	6.12	1.56	1.47
1	P	301	GLY	N-CA	-5.54	1.40	1.45
1	P	63	TYR	N-CA	-5.30	1.39	1.45
1	P	490	HIS	N-CA	-5.11	1.40	1.46
1	P	279	THR	CA-C	5.10	1.58	1.53

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	494	THR	CA-C-O	-15.71	105.89	120.34
1	P	179	ILE	CA-CB-CG2	14.60	135.32	110.50
1	P	494	THR	O-C-N	14.12	131.96	121.65
1	P	177	VAL	N-CA-CB	-13.70	92.04	111.21
1	P	496	ARG	CA-C-O	-12.22	108.88	119.76
1	P	236	GLN	OE1-CD-NE2	10.68	133.28	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	489	CYS	CA-C-N	10.30	137.36	123.46
1	P	489	CYS	C-N-CA	10.30	137.36	123.46
1	P	279	THR	CA-CB-OG1	10.12	124.78	109.60
1	P	80	ARG	NE-CZ-NH2	9.34	127.61	119.20
1	P	384	ARG	CD-NE-CZ	-9.32	111.35	124.40
1	P	327	THR	CB-CA-C	-9.05	93.41	109.71
1	P	424	GLU	CA-C-O	-8.93	107.93	120.16
1	P	291	ARG	NE-CZ-NH2	-8.68	111.39	119.20
1	P	299	ARG	NE-CZ-NH1	-8.22	113.28	121.50
1	P	242	SER	N-CA-C	-8.07	98.53	110.48
1	P	62	PHE	O-C-N	-8.06	113.01	123.16
1	P	405	HIS	CA-CB-CG	-8.04	105.76	113.80
1	P	107	VAL	CB-CA-C	-8.03	99.25	112.26
1	P	291	ARG	NE-CZ-NH1	8.03	129.53	121.50
1	P	333	SER	CA-C-O	7.97	129.11	120.10
1	P	311	ARG	CD-NE-CZ	7.66	135.12	124.40
1	P	299	ARG	NH1-CZ-NH2	7.65	129.24	119.30
1	P	190	GLN	OE1-CD-NE2	-7.55	115.05	122.60
1	P	179	ILE	N-CA-CB	-7.50	100.71	111.21
1	P	378	SER	CB-CA-C	-7.47	98.39	110.79
1	P	355	GLY	O-C-N	-7.45	117.11	123.59
1	P	136	PRO	N-CA-C	7.44	119.78	110.70
1	P	372	SER	CA-CB-OG	-7.44	96.22	111.10
1	P	215	GLN	OE1-CD-NE2	-7.44	115.16	122.60
1	P	206	HIS	CA-CB-CG	-7.41	106.39	113.80
1	P	51	GLN	CB-CG-CD	-7.41	100.01	112.60
1	P	150	SER	N-CA-CB	7.40	120.94	110.36
1	P	149	TYR	CA-C-O	-7.40	113.39	120.56
1	P	496	ARG	O-C-N	7.32	129.18	121.42
1	P	279	THR	CB-CA-C	-7.31	97.60	114.41
1	P	329	GLU	CA-CB-CG	-7.26	99.57	114.10
1	P	194	LEU	O-C-N	-7.23	113.92	120.71
1	P	254	LEU	CB-CA-C	-7.15	99.66	110.88
1	P	114	ARG	CA-C-O	7.09	127.85	119.48
1	P	123	LYS	CA-C-O	-7.08	112.62	120.69
1	P	171	GLY	N-CA-C	7.05	124.37	115.42
1	P	166	THR	CA-C-O	7.03	129.80	120.16
1	P	73	ARG	NE-CZ-NH1	-7.02	114.48	121.50
1	P	73	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	P	319	PRO	CA-C-O	6.98	129.30	121.34
1	P	496	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	P	400	THR	CA-CB-OG1	6.85	119.88	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	226	HIS	CA-CB-CG	-6.84	106.96	113.80
1	P	367	LYS	CA-C-O	-6.79	113.27	121.89
1	P	287	MET	N-CA-CB	-6.77	98.81	110.32
1	P	381	ASP	O-C-N	-6.71	116.25	123.42
1	P	391	THR	OG1-CB-CG2	-6.68	95.94	109.30
1	P	221	LEU	CA-C-N	6.68	132.65	122.77
1	P	221	LEU	C-N-CA	6.68	132.65	122.77
1	P	359	SER	O-C-N	-6.63	114.47	120.71
1	P	97	ARG	CD-NE-CZ	6.53	133.54	124.40
1	P	489	CYS	CA-CB-SG	-6.51	99.43	114.40
1	P	326	VAL	CA-C-O	-6.50	113.63	120.39
1	P	291	ARG	CD-NE-CZ	6.49	133.49	124.40
1	P	239	ALA	CA-C-O	-6.47	113.26	120.70
1	P	67	SER	CB-CA-C	6.44	119.81	111.50
1	P	322	ILE	CA-C-O	-6.42	113.67	120.53
1	P	164	PRO	CA-C-N	-6.38	111.77	121.53
1	P	164	PRO	C-N-CA	-6.38	111.77	121.53
1	P	453	LEU	N-CA-CB	-6.38	100.75	110.12
1	P	442	LEU	O-C-N	-6.37	114.52	122.35
1	P	153	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	P	242	SER	CA-C-O	-6.34	114.18	121.47
1	P	27	PHE	CA-CB-CG	6.31	120.11	113.80
1	P	312	GLU	CB-CG-CD	-6.28	101.92	112.60
1	P	80	ARG	NE-CZ-NH1	-6.27	115.23	121.50
1	P	488	CYS	CA-C-N	6.26	133.49	121.54
1	P	488	CYS	C-N-CA	6.26	133.49	121.54
1	P	436	GLY	O-C-N	-6.26	115.58	122.84
1	P	279	THR	N-CA-CB	6.25	122.05	110.86
1	P	25	LEU	CA-C-O	-6.19	114.16	120.84
1	P	63	TYR	N-CA-C	6.17	118.79	109.23
1	P	119	GLY	O-C-N	-6.16	117.84	123.57
1	P	185	LEU	CA-C-N	-6.16	114.00	122.93
1	P	185	LEU	C-N-CA	-6.16	114.00	122.93
1	P	201	TYR	O-C-N	-6.12	115.63	122.12
1	P	292	GLY	CA-C-O	-6.11	115.91	121.47
1	P	184	ASN	OD1-CG-ND2	6.08	128.68	122.60
1	P	400	THR	N-CA-CB	-6.06	100.26	111.53
1	P	150	SER	CA-CB-OG	-6.06	98.99	111.10
1	P	249	ASP	CA-CB-CG	-6.05	106.55	112.60
1	P	290	SER	CA-CB-OG	-6.05	99.01	111.10
1	P	171	GLY	CA-C-O	-6.04	113.22	119.20
1	P	329	GLU	CB-CG-CD	-6.03	102.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	391	THR	N-CA-CB	5.99	120.53	110.77
1	P	424	GLU	O-C-N	5.97	128.19	121.32
1	P	486	GLN	CA-C-N	5.93	128.52	120.63
1	P	486	GLN	C-N-CA	5.93	128.52	120.63
1	P	494	THR	N-CA-CB	5.92	119.60	111.25
1	P	333	SER	O-C-N	-5.90	115.31	122.22
1	P	274	THR	N-CA-C	5.90	118.14	108.52
1	P	401	GLN	N-CA-CB	-5.89	101.00	110.77
1	P	85	MET	CA-CB-CG	-5.86	102.37	114.10
1	P	423	HIS	CA-CB-CG	-5.86	107.94	113.80
1	P	223	TYR	O-C-N	-5.85	115.49	122.63
1	P	153	GLN	O-C-N	-5.83	114.63	122.68
1	P	136	PRO	CA-C-N	5.81	126.21	119.47
1	P	136	PRO	C-N-CA	5.81	126.21	119.47
1	P	232	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	P	194	LEU	CA-C-O	5.78	123.94	118.34
1	P	438	ASN	OD1-CG-ND2	5.77	128.37	122.60
1	P	367	LYS	CA-C-N	-5.73	112.36	120.49
1	P	367	LYS	C-N-CA	-5.73	112.36	120.49
1	P	157	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	P	457	LYS	CA-C-O	-5.71	114.49	120.55
1	P	170	GLY	N-CA-C	5.71	122.95	115.47
1	P	295	SER	N-CA-C	-5.70	106.18	113.02
1	P	224	ALA	O-C-N	-5.69	114.87	122.38
1	P	33	TYR	CB-CG-CD1	-5.65	112.33	120.80
1	P	334	LEU	CA-C-O	5.64	126.31	119.49
1	P	22	ASN	OD1-CG-ND2	5.63	128.23	122.60
1	P	184	ASN	CA-CB-CG	-5.62	106.98	112.60
1	P	254	LEU	N-CA-C	-5.62	105.06	111.07
1	P	145	LEU	O-C-N	-5.58	115.75	123.12
1	P	263	THR	O-C-N	-5.54	116.04	122.03
1	P	404	ALA	CA-C-O	-5.54	113.84	120.10
1	P	39	TYR	N-CA-C	-5.53	105.75	112.88
1	P	284	PRO	N-CA-C	5.52	120.15	111.38
1	P	425	PRO	N-CA-CB	5.51	108.66	102.60
1	P	329	GLU	OE1-CD-OE2	5.49	136.08	122.90
1	P	389	VAL	CA-C-O	-5.49	114.52	120.67
1	P	115	GLY	N-CA-C	5.47	123.14	115.43
1	P	48	ASN	CA-CB-CG	-5.44	107.16	112.60
1	P	299	ARG	N-CA-CB	-5.44	101.57	110.43
1	P	193	TRP	CB-CG-CD1	5.43	135.05	126.90
1	P	391	THR	CA-CB-OG1	-5.42	101.47	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	80	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	P	451	GLU	CB-CG-CD	5.41	121.80	112.60
1	P	209	MET	CA-C-N	5.41	128.30	120.79
1	P	209	MET	C-N-CA	5.41	128.30	120.79
1	P	288	ARG	CG-CD-NE	-5.40	100.12	112.00
1	P	386	VAL	CA-CB-CG1	-5.39	101.24	110.40
1	P	327	THR	CA-C-N	5.38	130.83	122.49
1	P	327	THR	C-N-CA	5.38	130.83	122.49
1	P	152	ASP	CA-CB-CG	-5.38	107.22	112.60
1	P	267	ASP	CA-C-O	-5.38	112.82	120.51
1	P	334	LEU	O-C-N	-5.37	115.41	122.39
1	P	289	MET	CB-CA-C	-5.37	110.41	116.63
1	P	404	ALA	N-CA-C	-5.36	105.54	111.71
1	P	438	ASN	CA-CB-CG	5.35	117.95	112.60
1	P	312	GLU	CG-CD-OE1	5.34	130.69	118.40
1	P	226	HIS	N-CA-CB	5.33	118.33	110.33
1	P	413	ALA	CA-C-O	-5.33	112.82	119.38
1	P	226	HIS	N-CA-C	-5.33	105.92	112.90
1	P	442	LEU	N-CA-CB	-5.33	102.76	110.70
1	P	250	SER	N-CA-CB	-5.32	102.04	110.28
1	P	73	ARG	CD-NE-CZ	5.29	131.80	124.40
1	P	495	PRO	CA-N-CD	-5.27	104.12	111.50
1	P	359	SER	CA-C-O	5.26	123.44	118.34
1	P	411	ASP	CB-CA-C	5.25	117.92	109.51
1	P	112	ALA	N-CA-C	-5.25	105.47	111.14
1	P	177	VAL	CA-CB-CG1	5.23	119.28	110.40
1	P	497	PRO	CA-N-CD	-5.21	104.20	111.50
1	P	317	PHE	CA-CB-CG	5.21	119.01	113.80
1	P	401	GLN	CA-C-O	-5.21	114.42	120.31
1	P	37	GLY	CA-C-O	5.21	126.11	120.75
1	P	81	LEU	N-CA-C	-5.19	103.05	109.64
1	P	70	THR	CA-C-O	5.19	124.01	119.08
1	P	174	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	P	295	SER	CA-CB-OG	-5.18	100.74	111.10
1	P	161	CYS	N-CA-C	-5.18	107.09	113.41
1	P	271	LEU	N-CA-CB	5.18	119.24	110.49
1	P	496	ARG	CA-CB-CG	5.17	124.43	114.10
1	P	48	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	P	88	TYR	CA-C-O	-5.16	115.87	120.56
1	P	374	PHE	CA-CB-CG	-5.15	108.65	113.80
1	P	227	HIS	CA-CB-CG	-5.15	108.65	113.80
1	P	142	HIS	CA-CB-CG	-5.15	108.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	179	ILE	CB-CG1-CD1	-5.14	103.00	113.80
1	P	495	PRO	N-CD-CG	5.13	109.96	103.80
1	P	242	SER	CA-C-N	-5.13	111.35	121.41
1	P	242	SER	C-N-CA	-5.13	111.35	121.41
1	P	114	ARG	N-CA-C	-5.13	105.71	112.94
1	P	272	GLU	CA-C-O	-5.13	113.18	120.51
1	P	190	GLN	CG-CD-NE2	5.11	124.07	116.40
1	P	242	SER	O-C-N	-5.10	117.19	122.96
1	P	263	THR	CA-C-O	5.10	126.15	120.90
1	P	319	PRO	O-C-N	-5.10	116.86	123.03
1	P	332	SER	O-C-N	-5.09	116.53	123.15
1	P	488	CYS	O-C-N	-5.08	116.41	123.12
1	P	33	TYR	CA-C-O	-5.08	114.36	120.10
1	P	193	TRP	CB-CG-CD2	-5.06	119.71	126.80
1	P	118	THR	N-CA-C	5.05	117.21	109.07
1	P	407	ASP	CA-CB-CG	5.02	117.62	112.60
1	P	46	THR	O-C-N	-5.01	116.99	121.20
1	P	69	ALA	N-CA-C	5.00	116.42	110.97
1	P	326	VAL	O-C-N	-5.00	117.90	123.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	107	VAL	Mainchain
1	P	223	TYR	Mainchain
1	P	241	ARG	Mainchain
1	P	327	THR	Mainchain
1	P	442	LEU	Mainchain
1	P	54	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	3553	0	3421	91	1
2	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	93	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.

All (93) 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:CD	5:P:2038:HOH:O	2.16	0.89
1:P:109:GLU:OE2	5:P:2038:HOH:O	1.92	0.87
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
1:P:327:THR:HG23	5:P:2107:HOH:O	1.83	0.78
1:P:407:ASP:OD1	5:P:2134:HOH:O	2.10	0.69
1:P:19:ARG:N	1:P:20:PRO:HD2	2.09	0.67
1:P:150:SER:H	1:P:153:GLN:HE21	1.42	0.67
1:P:198:GLU:HB3	5:P:2063:HOH:O	1.95	0.65
1:P:198:GLU:CG	5:P:2070:HOH:O	2.45	0.65
1:P:358:LEU:HD22	1:P:369:PRO:HD2	1.78	0.65
1:P:386:VAL:HG11	1:P:466:LEU:CD2	2.27	0.64
1:P:198:GLU:HG3	5:P:2070:HOH:O	1.98	0.63
1:P:24:VAL:HG13	1:P:276:VAL:HG22	1.79	0.63
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.34	0.62
1:P:376:TYR:CZ	1:P:386:VAL:HG12	2.35	0.61
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.01	0.60
1:P:102:LEU:O	5:P:2034:HOH:O	2.17	0.60
1:P:327:THR:HG22	1:P:329:GLU:H	1.68	0.59
1:P:242:SER:HB3	1:P:252:MET:HE2	1.86	0.58
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.34	0.57
1:P:386:VAL:CG1	1:P:466:LEU:HD23	2.33	0.57
1:P:407:ASP:CG	5:P:2134:HOH:O	2.49	0.56
1:P:149:TYR:HB2	1:P:153:GLN:NE2	2.21	0.56
1:P:407:ASP:CB	5:P:2134:HOH:O	2.54	0.56
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.88	0.54
1:P:159:LEU:HD21	1:P:191:PRO:HG3	1.90	0.54
1:P:279:THR:HG23	1:P:313:PRO:O	2.07	0.53
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:117:LEU:HD23	1:P:212:ALA:HB2	1.90	0.53
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.22	0.52
1:P:123:LYS:NZ	1:P:150:SER:HB3	2.25	0.52
1:P:150:SER:H	1:P:153:GLN:NE2	2.05	0.51
1:P:215:GLN:HB2	1:P:217:ARG:HG2	1.93	0.51
1:P:378:SER:HB2	1:P:379:TYR:CD1	2.47	0.50
1:P:151:HIS:CD2	1:P:231:PRO:HD2	2.47	0.50
1:P:449:THR:HG22	1:P:451:GLU:H	1.76	0.50
1:P:378:SER:HB2	1:P:379:TYR:HD1	1.77	0.50
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.94	0.50
1:P:85:MET:HG3	1:P:87:MET:HG2	1.95	0.49
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.47	0.49
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.96	0.49
1:P:202:MET:SD	1:P:261:LEU:HD13	2.53	0.48
1:P:337:LEU:HB3	1:P:338:PRO:CD	2.42	0.48
1:P:502:CYS:SG	1:P:502:CYS:O	2.70	0.48
1:P:26:ILE:HD13	1:P:258:VAL:HG22	1.95	0.48
1:P:199:ALA:O	1:P:200:ARG:C	2.54	0.48
1:P:210:ALA:O	1:P:211:ASP:C	2.54	0.48
1:P:415:HIS:CD2	5:P:2136:HOH:O	2.68	0.47
1:P:264:ALA:O	1:P:268:LEU:HG	2.15	0.47
1:P:123:LYS:HZ1	1:P:150:SER:HB3	1.80	0.47
1:P:263:THR:O	1:P:264:ALA:C	2.56	0.47
1:P:312:GLU:HB3	1:P:313:PRO:HD2	1.97	0.47
1:P:236:GLN:O	1:P:236:GLN:HG3	2.15	0.47
1:P:190:GLN:HA	1:P:191:PRO:HA	1.68	0.46
1:P:152:ASP:O	1:P:172:CYS:HB3	2.16	0.46
1:P:154:GLY:O	1:P:172:CYS:HB2	2.16	0.46
1:P:150:SER:N	1:P:153:GLN:HE21	2.11	0.46
1:P:70:THR:N	1:P:71:PRO:HD2	2.31	0.45
1:P:400:THR:HG23	5:P:2138:HOH:O	2.16	0.45
1:P:440:ASN:ND2	1:P:442:LEU:H	2.15	0.45
1:P:449:THR:HG22	1:P:451:GLU:N	2.32	0.45
1:P:238:PHE:HB3	1:P:252:MET:HE3	1.97	0.45
1:P:279:THR:CG2	1:P:313:PRO:O	2.65	0.44
1:P:80:ARG:HB2	1:P:85:MET:HE1	1.99	0.44
1:P:332:SER:OG	1:P:334:LEU:HB2	2.18	0.44
1:P:482:ASP:HB3	1:P:485:LEU:HD22	1.99	0.44
1:P:415:HIS:HD2	5:P:2136:HOH:O	1.99	0.44
1:P:372:SER:HA	1:P:390:ARG:O	2.18	0.43
1:P:349:PRO:HB2	1:P:351:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:268:LEU:HB2	1:P:270:LEU:HG	2.01	0.43
1:P:135:LEU:HB3	1:P:136:PRO:HD2	2.00	0.43
1:P:268:LEU:N	1:P:268:LEU:HD23	2.33	0.43
1:P:159:LEU:HD21	1:P:191:PRO:CG	2.50	0.42
1:P:198:GLU:OE1	5:P:2064:HOH:O	2.22	0.42
1:P:279:THR:HG22	1:P:280:ALA:H	1.83	0.42
1:P:337:LEU:CB	1:P:338:PRO:CD	2.97	0.42
1:P:188:GLU:HG3	1:P:188:GLU:O	2.19	0.42
1:P:227:HIS:HA	1:P:228:THR:HA	1.75	0.42
1:P:410:ALA:O	1:P:412:PRO:HD3	2.20	0.42
1:P:123:LYS:HD2	1:P:150:SER:HA	2.02	0.41
1:P:327:THR:HG21	1:P:361:LEU:HD11	2.02	0.41
1:P:241:ARG:CB	1:P:252:MET:HE1	2.50	0.41
1:P:496:ARG:NH1	5:P:2164:HOH:O	2.53	0.41
1:P:384:ARG:HH11	1:P:384:ARG:HD3	1.49	0.41
1:P:430:ASP:OD2	1:P:433:LYS:HE2	2.20	0.41
1:P:88:TYR:HB2	1:P:89:PRO:HA	2.02	0.41
1:P:244:ARG:HG2	1:P:244:ARG:O	2.21	0.40
1:P:147:ILE:HD13	1:P:179:ILE:HG23	2.02	0.40
1:P:344:ALA:O	1:P:345:GLY:C	2.63	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]	2.10	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%)	43 52

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	369/384 (96%)	333 (90%)	36 (10%)	7 7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	VAL
1	P	52	LEU
1	P	85	MET
1	P	107	VAL
1	P	111	LEU
1	P	125	HIS
1	P	150	SER
1	P	161	CYS
1	P	177	VAL
1	P	179	ILE
1	P	188	GLU
1	P	197	LEU
1	P	198	GLU
1	P	217	ARG
1	P	236	GLN
1	P	237	SER
1	P	254	LEU
1	P	261	LEU
1	P	268	LEU
1	P	279	THR
1	P	282	ASN
1	P	287	MET
1	P	327	THR
1	P	334	LEU

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Mol	Chain	Res	Type
1	P	336	LEU
1	P	337	LEU
1	P	343	LEU
1	P	352	THR
1	P	362	LEU
1	P	377	PRO
1	P	382	GLU
1	P	400	THR
1	P	433	LYS
1	P	442	LEU
1	P	451	GLU
1	P	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	48	ASN
1	P	153	GLN
1	P	226	HIS
1	P	282	ASN
1	P	328	HIS
1	P	423	HIS
1	P	440	ASN
1	P	465	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	1.75	4 (28%)	17,19,21	3.79	11 (64%)
2	NAG	A	2	2	14,14,15	1.44	2 (14%)	17,19,21	2.04	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	3/6/23/26	0/1/1/1
2	NAG	A	2	2	1/1/5/7	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAG	O7-C7	-3.39	1.15	1.23
2	A	1	NAG	O7-C7	-3.34	1.15	1.23
2	A	1	NAG	C2-N2	3.15	1.51	1.46
2	A	1	NAG	O5-C5	-2.81	1.38	1.43
2	A	2	NAG	C2-N2	2.70	1.50	1.46
2	A	1	NAG	O4-C4	-2.13	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O7-C7-N2	-7.46	108.80	121.98
2	A	1	NAG	C8-C7-N2	7.43	128.45	116.12
2	A	1	NAG	O4-C4-C3	6.02	124.57	110.38
2	A	2	NAG	C1-O5-C5	5.92	120.11	112.19
2	A	1	NAG	O5-C1-C2	5.61	119.98	111.29
2	A	1	NAG	O4-C4-C5	-4.54	98.14	109.32
2	A	1	NAG	C1-O5-C5	3.67	117.11	112.19
2	A	2	NAG	C2-N2-C7	-3.55	118.14	122.90
2	A	2	NAG	C3-C4-C5	2.83	115.36	110.23
2	A	1	NAG	O3-C3-C2	2.69	114.99	109.40
2	A	2	NAG	O3-C3-C2	-2.67	103.85	109.40
2	A	1	NAG	C3-C4-C5	-2.30	106.07	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-C2-N2	2.20	113.90	110.43
2	A	1	NAG	C6-C5-C4	-2.20	107.62	113.02
2	A	1	NAG	O5-C5-C6	2.03	111.61	107.66

All (2) chirality outliers are listed below:

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

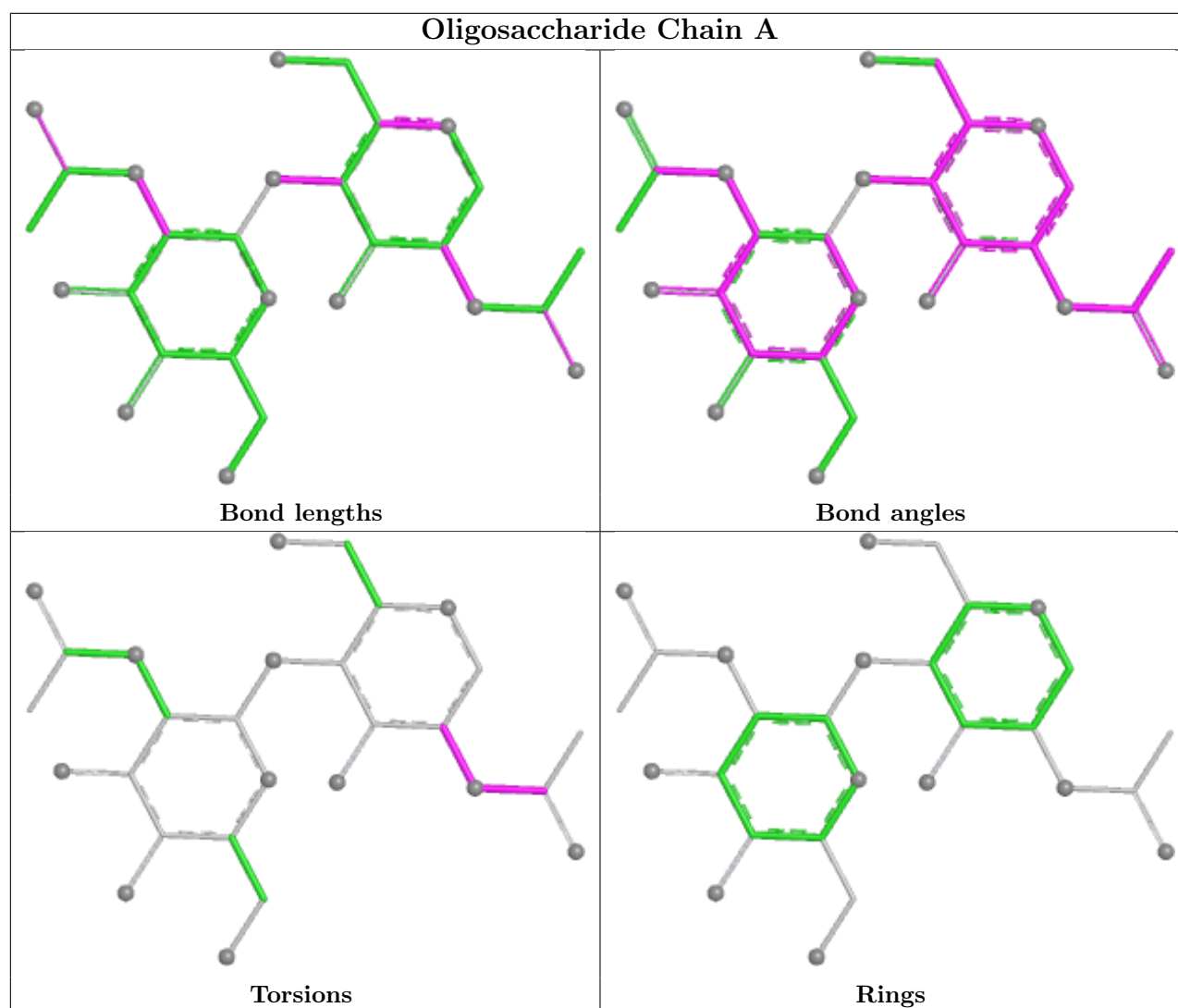
All (3) torsion outliers are listed below:

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



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]	-	15,15,15	1.37	3 (20%)	18,22,22	3.84	10 (55%)
4	CSN	P	701[B]	-	15,15,15	1.37	2 (13%)	18,22,22	2.65	11 (61%)

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	-3.71	1.28	1.36
4	P	701[A]	CSN	O7-C2	-3.01	1.30	1.36
4	P	701[A]	CSN	O4-S1	2.69	1.63	1.58
4	P	701[B]	CSN	O4-S1	2.69	1.63	1.58
4	P	701[A]	CSN	O4-C1	-2.55	1.37	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	701[A]	CSN	C4-C5-N1	9.89	127.97	119.34
4	P	701[A]	CSN	C6-C5-N1	-6.60	113.05	118.74
4	P	701[A]	CSN	C3-C2-C1	-6.16	112.57	119.55
4	P	701[A]	CSN	C6-C1-C2	5.52	125.61	120.04
4	P	701[B]	CSN	C6-C1-C2	4.70	124.78	120.04
4	P	701[B]	CSN	C6-C5-N1	-4.66	114.72	118.74
4	P	701[A]	CSN	O6-N1-C5	3.92	124.21	118.82
4	P	701[B]	CSN	C5-C6-C1	-3.91	114.83	119.06
4	P	701[B]	CSN	O7-C2-C1	3.88	129.25	120.13
4	P	701[A]	CSN	O7-C2-C3	3.12	127.74	119.36
4	P	701[A]	CSN	O4-S1-O3	-2.96	98.53	107.56
4	P	701[B]	CSN	O4-S1-O3	-2.96	98.53	107.56
4	P	701[B]	CSN	C4-C5-C6	2.80	123.72	120.11
4	P	701[A]	CSN	C4-C3-C2	2.72	123.22	120.50
4	P	701[B]	CSN	C4-C5-N1	2.52	121.53	119.34
4	P	701[A]	CSN	O4-C1-C2	-2.40	115.12	118.00
4	P	701[B]	CSN	C3-C2-C1	-2.38	116.85	119.55
4	P	701[A]	CSN	O1-S1-O2	2.34	116.73	108.56
4	P	701[B]	CSN	O1-S1-O2	2.34	116.73	108.56
4	P	701[B]	CSN	O4-C1-C6	-2.30	114.86	118.80
4	P	701[B]	CSN	O7-C2-C3	-2.04	113.89	119.36

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 [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%)	-0.02	7 (1%) 72 77	23, 40, 65, 86	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	448	ALA	6.9
1	P	503	PRO	5.0
1	P	198	GLU	4.5
1	P	490	HIS	3.9
1	P	19	ARG	2.2
1	P	501	HIS	2.2
1	P	449	THR	2.1

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

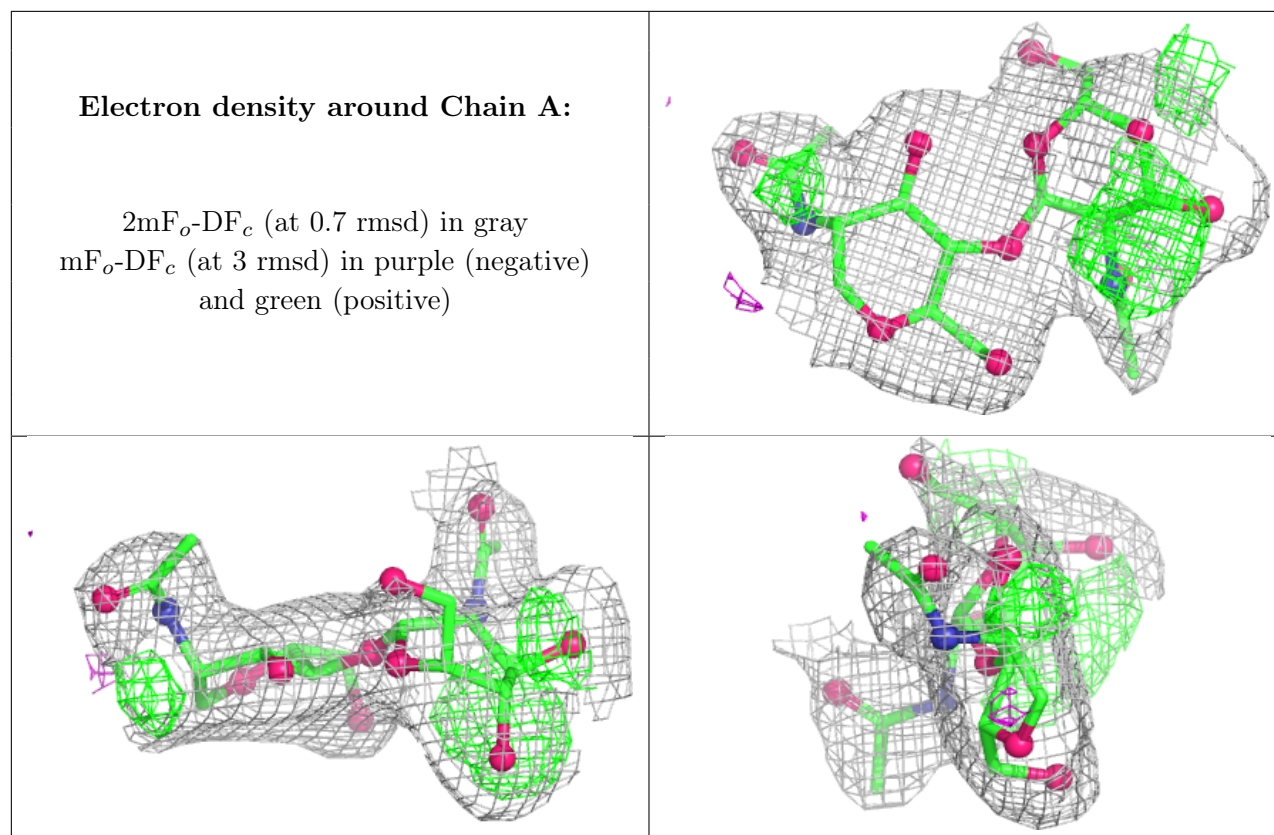
There are no non-standard protein/DNA/RNA residues in this entry.

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	-	-	51,63,72,78	0
2	NAG	A	2	14/15	-	-	82,89,95,98	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
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.