



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:26 PM UTC

PDB ID : 1E33 / pdb_00001e33
Title : Crystal structure of an Arylsulfatase A mutant P426L
Authors : von Buelow, R.; Schmidt, B.; Dierks, T.; von Figura, K.; Uson, I.
Deposited on : 2000-06-06
Resolution : 2.50 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

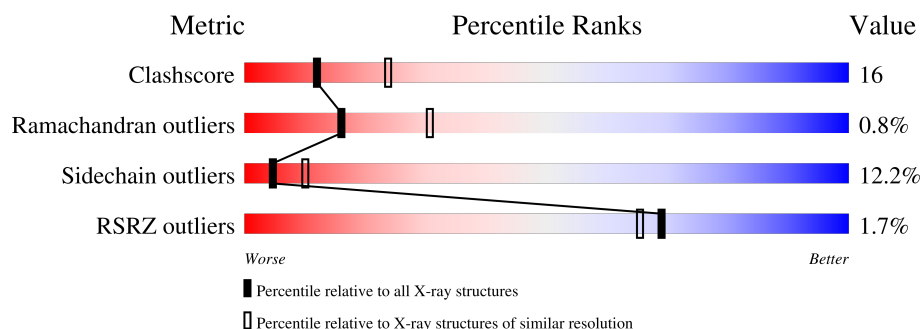
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

There are 4 unique types of molecules in this entry. The entry contains 3754 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
			3555	2269	602	661	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	215	GLU	GLN	conflict	UNP P15289
P	426	LEU	PRO	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	170	Total	O	0	0
			170	170		

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.40Å 131.40Å 192.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.50) 99.0 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.250 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.7	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	3754	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, DDZ, 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	1.33	8/3653 (0.2%)	2.73	362/4991 (7.3%)

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	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	490	HIS	N-CA	-8.29	1.37	1.46
1	P	502	CYS	C-O	-7.32	1.14	1.24
1	P	301	GLY	N-CA	-6.96	1.39	1.46
1	P	503	PRO	N-CD	6.57	1.56	1.47
1	P	151	HIS	CG-ND1	6.22	1.45	1.38
1	P	131	GLU	C-N	5.56	1.40	1.33
1	P	243	GLY	N-CA	5.54	1.53	1.45
1	P	279	THR	CA-C	5.16	1.59	1.53

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	489	CYS	CA-C-N	17.56	144.40	123.15
1	P	489	CYS	C-N-CA	17.56	144.40	123.15
1	P	494	THR	O-C-N	16.45	134.66	121.83
1	P	494	THR	CA-C-O	-15.10	105.11	119.76
1	P	73	ARG	CD-NE-CZ	14.60	144.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	291	ARG	NE-CZ-NH2	-14.03	106.57	119.20
1	P	244	ARG	NE-CZ-NH1	12.60	134.10	121.50
1	P	179	ILE	CA-CB-CG2	12.39	131.57	110.50
1	P	288	ARG	NE-CZ-NH2	11.96	129.96	119.20
1	P	300	CYS	CA-C-N	11.95	131.36	122.16
1	P	300	CYS	C-N-CA	11.95	131.36	122.16
1	P	496	ARG	CA-C-O	-11.71	108.09	119.80
1	P	177	VAL	N-CA-CB	-11.57	95.01	111.21
1	P	242	SER	CA-C-O	-11.38	108.39	121.47
1	P	244	ARG	NH1-CZ-NH2	-11.34	104.56	119.30
1	P	22	ASN	OD1-CG-ND2	11.07	133.67	122.60
1	P	496	ARG	CD-NE-CZ	10.89	139.65	124.40
1	P	249	ASP	CA-CB-CG	-10.74	101.86	112.60
1	P	352	THR	CA-C-N	10.56	138.25	122.93
1	P	352	THR	C-N-CA	10.56	138.25	122.93
1	P	171	GLY	N-CA-C	10.42	128.65	115.42
1	P	184	ASN	OD1-CG-ND2	9.86	132.46	122.60
1	P	239	ALA	CA-C-O	-9.82	110.20	120.80
1	P	391	THR	OG1-CB-CG2	-9.81	89.68	109.30
1	P	391	THR	CA-CB-OG1	-9.79	94.91	109.60
1	P	327	THR	CB-CA-C	-9.62	91.77	109.37
1	P	114	ARG	N-CA-C	-9.53	100.58	112.88
1	P	429	TYR	O-C-N	9.23	134.59	123.24
1	P	88	TYR	O-C-N	9.18	130.65	121.56
1	P	73	ARG	NE-CZ-NH1	-9.02	112.48	121.50
1	P	143	ARG	CD-NE-CZ	8.96	136.94	124.40
1	P	81	LEU	CA-C-O	8.79	129.32	120.17
1	P	127	GLY	CA-C-O	8.76	127.92	122.22
1	P	344	ALA	CA-C-O	8.71	129.87	119.59
1	P	279	THR	CB-CA-C	-8.66	93.90	112.78
1	P	33	TYR	CA-C-O	-8.61	110.56	120.20
1	P	311	ARG	CD-NE-CZ	8.60	136.44	124.40
1	P	62	PHE	O-C-N	-8.58	113.15	123.19
1	P	97	ARG	NE-CZ-NH2	8.57	126.91	119.20
1	P	149	TYR	CA-C-O	-8.50	112.10	120.94
1	P	398	PHE	CA-CB-CG	-8.46	105.34	113.80
1	P	170	GLY	CA-C-N	-8.46	109.68	122.28
1	P	170	GLY	C-N-CA	-8.46	109.68	122.28
1	P	166	THR	CA-C-O	8.44	125.96	119.46
1	P	41	HIS	CA-CB-CG	-8.44	105.36	113.80
1	P	109	GLU	OE1-CD-OE2	-8.38	102.80	122.90
1	P	494	THR	N-CA-CB	8.34	122.36	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	320	GLY	CA-C-O	-8.30	110.99	119.20
1	P	344	ALA	O-C-N	-8.29	112.39	122.25
1	P	197	LEU	O-C-N	-8.27	113.49	122.09
1	P	158	ASN	OD1-CG-ND2	-8.21	114.39	122.60
1	P	397	HIS	CA-CB-CG	8.19	121.99	113.80
1	P	88	TYR	CA-C-O	-8.16	113.14	120.56
1	P	143	ARG	NE-CZ-NH2	-8.13	111.89	119.20
1	P	424	GLU	CA-C-O	-8.10	109.06	120.16
1	P	242	SER	CA-C-N	-8.05	105.62	121.41
1	P	242	SER	C-N-CA	-8.05	105.62	121.41
1	P	138	HIS	CA-CB-CG	-7.82	105.98	113.80
1	P	425	PRO	N-CA-CB	7.78	111.16	102.60
1	P	190	GLN	CG-CD-NE2	7.74	128.00	116.40
1	P	88	TYR	CB-CA-C	-7.73	101.33	110.76
1	P	314	ALA	CB-CA-C	7.71	122.93	109.89
1	P	267	ASP	CA-C-O	-7.67	109.55	120.51
1	P	442	LEU	N-CA-C	-7.63	103.53	112.92
1	P	351	VAL	O-C-N	7.60	131.48	123.04
1	P	226	HIS	CA-CB-CG	-7.58	106.22	113.80
1	P	267	ASP	CA-CB-CG	-7.57	105.03	112.60
1	P	440	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	P	39	TYR	N-CA-CB	7.55	123.00	110.92
1	P	501	HIS	CA-CB-CG	7.52	121.32	113.80
1	P	279	THR	N-CA-CB	7.49	122.65	110.97
1	P	211	ASP	O-C-N	-7.48	113.50	122.11
1	P	80	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	P	210	ALA	O-C-N	-7.41	114.15	122.08
1	P	287	MET	N-CA-CB	-7.40	97.74	110.32
1	P	247	PHE	CA-CB-CG	-7.38	106.42	113.80
1	P	319	PRO	CA-C-O	7.36	129.68	121.36
1	P	140	GLY	O-C-N	7.34	130.64	122.50
1	P	210	ALA	CB-CA-C	7.33	122.58	110.92
1	P	404	ALA	CA-C-O	-7.30	110.65	119.49
1	P	31	LEU	CA-C-N	-7.29	113.84	122.16
1	P	31	LEU	C-N-CA	-7.29	113.84	122.16
1	P	194	LEU	CA-C-O	-7.22	111.34	118.34
1	P	22	ASN	CB-CG-ND2	-7.21	105.59	116.40
1	P	81	LEU	O-C-N	-7.17	113.92	121.30
1	P	190	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	P	52	LEU	N-CA-CB	-7.14	98.53	110.39
1	P	454	GLN	CA-C-O	-7.12	112.87	120.42
1	P	281	ASP	CA-CB-CG	7.11	119.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	348	LEU	CA-C-O	7.09	127.46	120.23
1	P	221	LEU	O-C-N	-7.07	115.28	123.27
1	P	112	ALA	N-CA-C	-7.04	103.54	111.07
1	P	217	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	P	496	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	P	282	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	P	157	GLN	OE1-CD-NE2	-6.96	115.64	122.60
1	P	279	THR	CA-CB-OG1	6.94	120.01	109.60
1	P	426	LEU	N-CA-CB	-6.90	98.83	110.49
1	P	299	ARG	NH1-CZ-NH2	6.87	128.23	119.30
1	P	311	ARG	CG-CD-NE	6.85	127.08	112.00
1	P	151	HIS	CA-CB-CG	6.82	120.62	113.80
1	P	400	THR	N-CA-CB	-6.82	99.69	111.55
1	P	238	PHE	CA-CB-CG	-6.80	107.00	113.80
1	P	299	ARG	NE-CZ-NH1	-6.79	114.72	121.50
1	P	499	CYS	CA-C-N	-6.77	111.49	121.24
1	P	499	CYS	C-N-CA	-6.77	111.49	121.24
1	P	285	GLU	CA-C-O	6.75	128.95	121.39
1	P	263	THR	CA-C-O	6.69	127.59	120.70
1	P	330	LEU	O-C-N	-6.69	114.64	122.87
1	P	153	GLN	OE1-CD-NE2	-6.66	115.94	122.60
1	P	247	PHE	CA-C-O	6.64	127.61	119.97
1	P	291	ARG	NH1-CZ-NH2	6.64	127.93	119.30
1	P	489	CYS	CA-CB-SG	-6.62	99.18	114.40
1	P	48	ASN	CA-CB-CG	-6.60	106.00	112.60
1	P	140	GLY	CA-C-N	-6.60	113.61	122.72
1	P	140	GLY	C-N-CA	-6.60	113.61	122.72
1	P	223	TYR	O-C-N	-6.60	114.58	122.63
1	P	329	GLU	CB-CG-CD	-6.59	101.40	112.60
1	P	490	HIS	N-CA-CB	6.57	121.37	110.99
1	P	468	ALA	O-C-N	-6.55	114.21	122.27
1	P	108	ALA	CB-CA-C	6.54	121.97	110.85
1	P	251	LEU	CA-C-N	6.53	129.02	120.28
1	P	251	LEU	C-N-CA	6.53	129.02	120.28
1	P	242	SER	N-CA-C	-6.51	100.85	110.48
1	P	174	GLN	CG-CD-NE2	6.47	126.10	116.40
1	P	489	CYS	N-CA-C	6.45	120.01	111.75
1	P	488	CYS	N-CA-C	6.45	118.92	108.34
1	P	385	GLY	CA-C-O	-6.41	114.39	122.01
1	P	108	ALA	CA-C-N	6.39	129.68	120.79
1	P	108	ALA	C-N-CA	6.39	129.68	120.79
1	P	179	ILE	CA-CB-CG1	-6.38	99.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	497	PRO	CA-N-CD	-6.38	102.56	111.50
1	P	489	CYS	O-C-N	-6.37	114.94	122.20
1	P	151	HIS	ND1-CE1-NE2	6.34	114.75	108.40
1	P	361	LEU	CA-C-O	-6.30	114.21	120.82
1	P	351	VAL	CA-C-N	-6.29	112.50	121.50
1	P	351	VAL	C-N-CA	-6.29	112.50	121.50
1	P	109	GLU	CG-CD-OE1	6.29	132.86	118.40
1	P	244	ARG	CD-NE-CZ	-6.29	115.59	124.40
1	P	88	TYR	N-CA-C	-6.29	102.47	108.07
1	P	442	LEU	O-C-N	-6.29	114.80	122.34
1	P	77	LEU	CA-C-O	-6.27	112.39	119.79
1	P	390	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	P	41	HIS	N-CA-C	6.26	116.80	109.60
1	P	376	TYR	CA-CB-CG	6.26	125.17	113.90
1	P	235	GLY	CA-C-N	6.23	129.25	120.28
1	P	235	GLY	C-N-CA	6.23	129.25	120.28
1	P	154	GLY	N-CA-C	-6.22	99.64	112.34
1	P	288	ARG	NH1-CZ-NH2	-6.22	111.22	119.30
1	P	84	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	P	333	SER	N-CA-C	-6.20	104.58	111.71
1	P	329	GLU	CA-CB-CG	-6.19	101.71	114.10
1	P	51	GLN	CB-CG-CD	-6.19	102.08	112.60
1	P	328	HIS	CA-C-N	-6.19	111.23	120.94
1	P	328	HIS	C-N-CA	-6.19	111.23	120.94
1	P	475	SER	CA-C-N	6.18	128.85	120.44
1	P	475	SER	C-N-CA	6.18	128.85	120.44
1	P	102	LEU	O-C-N	6.17	129.86	122.27
1	P	185	LEU	CA-C-N	-6.17	113.69	122.94
1	P	185	LEU	C-N-CA	-6.17	113.69	122.94
1	P	351	VAL	CB-CA-C	-6.16	101.19	110.55
1	P	482	ASP	CA-C-N	6.16	126.34	119.32
1	P	482	ASP	C-N-CA	6.16	126.34	119.32
1	P	390	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	P	197	LEU	N-CA-CB	-6.12	100.81	109.94
1	P	249	ASP	N-CA-C	-6.10	104.54	111.07
1	P	469	ALA	N-CA-C	6.10	120.79	113.23
1	P	473	GLY	CA-C-N	6.09	126.41	119.83
1	P	473	GLY	C-N-CA	6.09	126.41	119.83
1	P	179	ILE	CB-CG1-CD1	-6.09	101.01	113.80
1	P	327	THR	OG1-CB-CG2	6.08	121.46	109.30
1	P	132	GLY	CA-C-O	6.08	127.28	119.68
1	P	154	GLY	CA-C-O	-6.08	112.83	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	301	GLY	CA-C-O	6.06	128.12	120.54
1	P	287	MET	O-C-N	-6.06	114.52	122.39
1	P	325	GLY	CA-C-N	6.04	131.45	123.11
1	P	325	GLY	C-N-CA	6.04	131.45	123.11
1	P	211	ASP	CA-C-N	6.03	128.37	120.28
1	P	211	ASP	C-N-CA	6.03	128.37	120.28
1	P	465	GLN	O-C-N	6.03	128.60	122.09
1	P	498	ALA	N-CA-C	6.03	118.64	111.71
1	P	116	TYR	CA-CB-CG	6.02	124.74	113.90
1	P	227	HIS	CA-CB-CG	-6.01	107.78	113.80
1	P	429	TYR	CA-C-N	-5.99	114.61	123.11
1	P	429	TYR	C-N-CA	-5.99	114.61	123.11
1	P	352	THR	CA-C-O	5.97	127.50	120.69
1	P	188	GLU	O-C-N	-5.97	114.22	122.46
1	P	231	PRO	CA-C-N	-5.96	111.49	121.39
1	P	231	PRO	C-N-CA	-5.96	111.49	121.39
1	P	263	THR	O-C-N	-5.95	115.66	122.09
1	P	378	SER	CB-CA-C	-5.95	100.91	110.79
1	P	352	THR	CB-CA-C	5.95	119.54	109.84
1	P	323	ALA	CA-C-O	5.95	126.30	120.23
1	P	493	CYS	CA-C-O	5.92	128.98	120.51
1	P	155	PRO	CA-C-O	-5.92	114.21	121.31
1	P	472	PHE	CA-CB-CG	5.91	119.71	113.80
1	P	104	GLU	N-CA-C	-5.90	102.19	110.50
1	P	111	LEU	CA-C-N	5.89	128.10	120.44
1	P	111	LEU	C-N-CA	5.89	128.10	120.44
1	P	219	PHE	O-C-N	-5.88	116.38	123.03
1	P	405	HIS	CA-CB-CG	-5.88	107.92	113.80
1	P	80	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	P	437	GLU	CA-CB-CG	5.87	125.84	114.10
1	P	226	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	P	86	GLY	CA-C-O	-5.84	111.77	119.25
1	P	109	GLU	CB-CG-CD	5.83	122.51	112.60
1	P	401	GLN	CA-C-O	-5.82	112.19	120.51
1	P	291	ARG	N-CA-C	-5.81	106.10	112.72
1	P	84	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	P	276	VAL	CB-CA-C	-5.80	102.58	110.42
1	P	63	TYR	N-CA-C	5.78	118.20	109.41
1	P	116	TYR	CA-C-N	-5.78	113.38	121.99
1	P	116	TYR	C-N-CA	-5.78	113.38	121.99
1	P	46	THR	CA-C-N	5.78	125.46	119.05
1	P	46	THR	C-N-CA	5.78	125.46	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	418	SER	N-CA-CB	5.76	118.59	110.24
1	P	235	GLY	N-CA-C	-5.75	103.59	112.85
1	P	97	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	P	257	ALA	O-C-N	-5.73	116.05	122.12
1	P	274	THR	N-CA-C	5.72	117.84	108.52
1	P	434	ASP	N-CA-CB	-5.72	101.95	110.99
1	P	177	VAL	CA-CB-CG1	5.71	120.11	110.40
1	P	502	CYS	O-C-N	5.70	127.87	121.32
1	P	81	LEU	N-CA-C	-5.68	102.42	109.64
1	P	170	GLY	N-CA-C	5.68	126.63	113.18
1	P	221	LEU	CA-C-N	5.67	131.53	123.14
1	P	221	LEU	C-N-CA	5.67	131.53	123.14
1	P	145	LEU	O-C-N	-5.66	115.65	123.12
1	P	443	GLY	CA-C-O	5.65	132.66	120.80
1	P	43	SER	N-CA-CB	5.65	120.04	111.06
1	P	426	LEU	CA-CB-CG	5.64	136.05	116.30
1	P	243	GLY	O-C-N	-5.64	115.37	122.70
1	P	23	ILE	N-CA-C	5.63	115.97	107.75
1	P	205	ALA	CA-C-O	-5.63	115.10	120.90
1	P	206	HIS	CA-CB-CG	-5.62	108.18	113.80
1	P	294	CYS	CA-C-O	-5.62	114.08	120.32
1	P	39	TYR	CA-C-N	-5.58	115.54	123.08
1	P	39	TYR	C-N-CA	-5.58	115.54	123.08
1	P	160	THR	CA-CB-OG1	-5.58	101.23	109.60
1	P	491	PRO	O-C-N	-5.57	115.91	122.99
1	P	260	THR	O-C-N	-5.57	116.33	122.07
1	P	374	PHE	CA-CB-CG	-5.57	108.23	113.80
1	P	479	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	P	26	ILE	CA-CB-CG1	-5.57	100.94	110.40
1	P	436	GLY	O-C-N	-5.57	115.02	122.48
1	P	272	GLU	CA-C-N	-5.56	113.62	122.29
1	P	272	GLU	C-N-CA	-5.56	113.62	122.29
1	P	309	GLY	O-C-N	5.53	129.88	122.70
1	P	179	ILE	N-CA-CB	-5.52	103.49	111.21
1	P	96	SER	CA-C-O	-5.51	114.85	120.80
1	P	33	TYR	CB-CG-CD2	-5.51	112.54	120.80
1	P	231	PRO	N-CA-CB	5.51	108.66	102.60
1	P	58	ARG	CA-C-N	-5.50	113.96	122.09
1	P	58	ARG	C-N-CA	-5.50	113.96	122.09
1	P	328	HIS	N-CA-C	-5.48	105.81	112.88
1	P	200	ARG	NE-CZ-NH2	-5.47	114.27	119.20
1	P	271	LEU	N-CA-C	5.46	117.66	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	481	GLU	CB-CG-CD	-5.46	103.32	112.60
1	P	160	THR	CA-C-N	-5.45	112.34	122.09
1	P	160	THR	C-N-CA	-5.45	112.34	122.09
1	P	193	TRP	CB-CG-CD1	5.45	135.07	126.90
1	P	132	GLY	N-CA-C	-5.44	105.51	114.76
1	P	140	GLY	CA-C-O	-5.44	113.08	118.96
1	P	33	TYR	CB-CG-CD1	5.43	128.95	120.80
1	P	161	CYS	CB-CA-C	5.43	118.74	109.24
1	P	492	GLY	CA-C-O	-5.42	113.58	118.95
1	P	337	LEU	CA-CB-CG	5.42	135.28	116.30
1	P	496	ARG	O-C-N	5.42	126.70	121.28
1	P	369	PRO	CB-CA-C	-5.42	103.77	111.68
1	P	366	GLY	CA-C-O	5.40	126.84	121.60
1	P	193	TRP	CB-CG-CD2	-5.40	119.24	126.80
1	P	485	LEU	CA-C-N	-5.40	113.21	120.82
1	P	485	LEU	C-N-CA	-5.40	113.21	120.82
1	P	37	GLY	CA-C-O	5.40	126.31	120.75
1	P	433	LYS	O-C-N	5.38	129.57	122.36
1	P	158	ASN	CB-CA-C	5.36	119.05	110.09
1	P	408	THR	CA-CB-OG1	5.36	117.64	109.60
1	P	308	GLY	O-C-N	-5.36	116.64	122.54
1	P	426	LEU	CA-C-N	5.35	129.15	121.50
1	P	426	LEU	C-N-CA	5.35	129.15	121.50
1	P	219	PHE	CA-C-N	5.33	130.63	122.95
1	P	219	PHE	C-N-CA	5.33	130.63	122.95
1	P	111	LEU	CA-C-O	5.33	125.50	119.27
1	P	352	THR	O-C-N	-5.33	116.81	123.04
1	P	449	THR	CA-CB-OG1	-5.33	101.61	109.60
1	P	160	THR	CA-CB-CG2	5.31	119.52	110.50
1	P	85	MET	CB-CA-C	-5.30	102.59	111.13
1	P	439	TYR	CB-CG-CD2	5.29	128.74	120.80
1	P	51	GLN	CA-CB-CG	5.27	124.63	114.10
1	P	118	THR	CA-C-N	-5.26	116.46	121.46
1	P	118	THR	C-N-CA	-5.26	116.46	121.46
1	P	210	ALA	CA-C-O	-5.25	115.29	121.07
1	P	463	LYS	O-C-N	-5.25	116.17	122.15
1	P	118	THR	N-CA-C	5.25	117.79	109.24
1	P	164	PRO	CA-C-N	-5.24	112.49	121.08
1	P	164	PRO	C-N-CA	-5.24	112.49	121.08
1	P	368	SER	N-CA-C	-5.24	103.44	109.93
1	P	154	GLY	CA-C-N	5.23	124.99	119.76
1	P	154	GLY	C-N-CA	5.23	124.99	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	146	GLY	N-CA-C	5.23	118.77	111.19
1	P	177	VAL	O-C-N	-5.23	115.14	121.10
1	P	276	VAL	CA-C-O	5.23	125.55	120.27
1	P	326	VAL	CG1-CB-CG2	-5.23	99.30	110.80
1	P	218	PRO	CA-C-N	-5.22	113.24	122.74
1	P	218	PRO	C-N-CA	-5.22	113.24	122.74
1	P	295	SER	CA-CB-OG	-5.22	100.66	111.10
1	P	52	LEU	O-C-N	-5.21	115.44	122.43
1	P	495	PRO	CA-N-CD	-5.21	104.20	111.50
1	P	109	GLU	O-C-N	-5.21	116.50	122.08
1	P	66	VAL	CA-C-O	-5.21	114.75	120.43
1	P	217	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	P	299	ARG	N-CA-CB	-5.20	101.58	110.16
1	P	62	PHE	CB-CA-C	5.19	118.20	109.48
1	P	321	HIS	CA-CB-CG	-5.19	108.61	113.80
1	P	52	LEU	CB-CA-C	5.18	121.14	110.31
1	P	62	PHE	CA-C-O	5.18	126.56	120.80
1	P	216	ASP	CA-C-O	-5.18	115.53	121.54
1	P	322	ILE	CA-C-O	-5.18	115.04	120.27
1	P	325	GLY	CA-C-O	5.18	126.82	121.38
1	P	330	LEU	CA-C-O	5.18	126.89	121.19
1	P	181	LEU	CA-C-N	5.17	131.19	122.87
1	P	181	LEU	C-N-CA	5.17	131.19	122.87
1	P	486	GLN	CA-C-N	5.16	127.62	120.49
1	P	486	GLN	C-N-CA	5.16	127.62	120.49
1	P	200	ARG	CD-NE-CZ	5.16	131.62	124.40
1	P	402	GLY	O-C-N	-5.15	116.22	122.71
1	P	106	THR	O-C-N	5.14	128.57	122.20
1	P	156	CYS	N-CA-C	-5.13	105.08	113.19
1	P	309	GLY	CA-C-O	-5.13	111.64	120.57
1	P	124	TRP	O-C-N	-5.13	115.06	122.03
1	P	91	VAL	CA-C-O	-5.12	116.29	121.67
1	P	198	GLU	CA-C-N	5.12	127.45	120.54
1	P	198	GLU	C-N-CA	5.12	127.45	120.54
1	P	282	ASN	CB-CG-ND2	5.12	124.08	116.40
1	P	20	PRO	O-C-N	5.11	123.66	121.31
1	P	71	PRO	N-CD-CG	-5.10	95.55	103.20
1	P	218	PRO	CB-CA-C	5.10	117.99	111.21
1	P	401	GLN	N-CA-CB	-5.10	101.88	110.49
1	P	146	GLY	CA-C-O	5.08	126.24	121.41
1	P	151	HIS	CG-ND1-CE1	-5.06	100.69	109.30
1	P	331	ALA	CA-C-N	5.06	130.64	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	331	ALA	C-N-CA	5.06	130.64	122.29
1	P	489	CYS	CB-CA-C	-5.06	100.64	110.46
1	P	324	PRO	CB-CA-C	-5.06	103.21	111.56
1	P	428	LEU	CA-C-O	5.06	125.60	120.24
1	P	470	VAL	CA-C-O	-5.05	115.08	120.59
1	P	223	TYR	N-CA-CB	-5.05	102.15	110.53
1	P	502	CYS	N-CA-C	-5.05	98.65	109.81
1	P	151	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	P	295	SER	N-CA-C	-5.04	106.91	113.16
1	P	312	GLU	CG-CD-OE1	5.04	129.98	118.40
1	P	229	HIS	CA-C-N	5.03	127.64	120.49
1	P	229	HIS	C-N-CA	5.03	127.64	120.49
1	P	228	THR	CA-C-O	5.03	129.35	120.80
1	P	387	PHE	CA-C-O	-5.03	113.87	120.00
1	P	110	VAL	N-CA-C	5.02	116.35	110.62
1	P	116	TYR	N-CA-C	-5.02	102.08	110.17
1	P	20	PRO	CA-C-O	-5.02	117.29	120.90
1	P	465	GLN	CA-C-N	-5.02	113.62	120.44
1	P	465	GLN	C-N-CA	-5.02	113.62	120.44
1	P	379	TYR	O-C-N	-5.01	115.56	121.32
1	P	311	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	128	VAL	Mainchain
1	P	150	SER	Mainchain
1	P	256	ALA	Mainchain
1	P	327	THR	Mainchain
1	P	380	PRO	Mainchain
1	P	42	PRO	Mainchain
1	P	89	PRO	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	3555	0	3418	108	0
2	A	28	0	24	3	0
3	P	1	0	0	0	0
4	P	170	0	0	19	0
All	All	3754	0	3442	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (110) 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	4:P:2146:HOH:O	1.41	1.01
1:P:501:HIS:O	1:P:502:CYS:HB3	1.70	0.91
1:P:150:SER:H	1:P:153:GLN:HE21	1.17	0.86
1:P:124:TRP:C	4:P:2039:HOH:O	2.18	0.86
1:P:217:ARG:O	4:P:2067:HOH:O	1.96	0.83
1:P:109:GLU:OE1	4:P:2037:HOH:O	1.96	0.83
1:P:150:SER:H	1:P:153:GLN:NE2	1.77	0.82
1:P:449:THR:HG22	1:P:452:VAL:H	1.42	0.82
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.63	0.81
1:P:500:CYS:O	1:P:501:HIS:HB3	1.88	0.73
1:P:327:THR:HG21	1:P:361:LEU:HD11	1.71	0.72
1:P:482:ASP:HB3	1:P:485:LEU:HD22	1.73	0.70
1:P:124:TRP:O	4:P:2039:HOH:O	2.07	0.70
1:P:124:TRP:CA	4:P:2039:HOH:O	2.41	0.66
1:P:327:THR:CG2	1:P:361:LEU:HD11	2.26	0.66
1:P:357:ASP:OD2	4:P:2116:HOH:O	2.14	0.65
1:P:151:HIS:CD2	1:P:231:PRO:HD2	2.32	0.65
1:P:393:LYS:NZ	4:P:2132:HOH:O	2.30	0.65
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.10	0.65
1:P:210:ALA:O	1:P:211:ASP:C	2.38	0.64
1:P:150:SER:N	1:P:153:GLN:HE21	1.91	0.64
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.81	0.64
1:P:102:LEU:O	4:P:2037:HOH:O	2.15	0.64
1:P:502:CYS:SG	1:P:502:CYS:O	2.55	0.64
1:P:213:GLN:O	1:P:214:ARG:C	2.42	0.63
1:P:188:GLU:HG3	1:P:188:GLU:O	1.98	0.62
1:P:449:THR:HG23	1:P:451:GLU:H	1.65	0.62
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.00	0.61
1:P:449:THR:CG2	1:P:451:GLU:H	2.15	0.60
1:P:198:GLU:CG	4:P:2069:HOH:O	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:202:MET:HA	1:P:202:MET:HE2	1.85	0.59
1:P:327:THR:HG22	1:P:329:GLU:H	1.65	0.59
2:A:1:NAG:H61	2:A:2:NAG:HN2	1.68	0.59
2:A:1:NAG:H61	2:A:2:NAG:N2	2.18	0.58
1:P:318:TRP:CB	1:P:322:ILE:HD12	2.35	0.57
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.34	0.56
1:P:260:THR:O	1:P:261:LEU:C	2.47	0.56
1:P:357:ASP:OD1	1:P:359:SER:OG	2.17	0.56
1:P:297:LEU:H	1:P:297:LEU:HD23	1.71	0.55
1:P:198:GLU:HG2	4:P:2069:HOH:O	2.07	0.55
1:P:124:TRP:HA	4:P:2039:HOH:O	2.05	0.54
1:P:111:LEU:O	1:P:116:TYR:HB2	2.06	0.54
1:P:156:CYS:HA	1:P:159:LEU:HG	1.88	0.54
1:P:129:GLY:O	4:P:2042:HOH:O	2.19	0.53
1:P:327:THR:HG23	4:P:2110:HOH:O	2.08	0.53
1:P:372:SER:HA	1:P:390:ARG:O	2.09	0.53
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.44	0.53
1:P:490:HIS:CG	1:P:493:CYS:HB3	2.44	0.52
1:P:19:ARG:CB	1:P:20:PRO:HD2	2.40	0.52
1:P:136:PRO:HG2	1:P:144:PHE:CD2	2.45	0.52
1:P:279:THR:HG23	1:P:313:PRO:O	2.11	0.51
1:P:152:ASP:O	1:P:172:CYS:HB3	2.10	0.51
1:P:163:PRO:HD3	1:P:195:PRO:HB3	1.92	0.51
1:P:202:MET:HG3	1:P:260:THR:HG21	1.93	0.51
1:P:318:TRP:HB3	1:P:322:ILE:HD12	1.93	0.51
1:P:93:VAL:O	1:P:96:SER:HB2	2.11	0.50
1:P:199:ALA:O	1:P:200:ARG:C	2.50	0.49
1:P:400:THR:HG21	1:P:423:HIS:HE1	1.77	0.49
1:P:70:THR:HB	1:P:71:PRO:CD	2.43	0.49
1:P:460:GLN:CD	4:P:2161:HOH:O	2.55	0.49
1:P:88:TYR:HB2	1:P:89:PRO:HA	1.94	0.49
1:P:22:ASN:OD1	1:P:218:PRO:HA	2.12	0.49
1:P:263:THR:O	1:P:264:ALA:C	2.52	0.49
1:P:202:MET:SD	1:P:261:LEU:HD13	2.53	0.49
1:P:188:GLU:OE2	1:P:200:ARG:NH2	2.46	0.48
1:P:20:PRO:HB2	1:P:116:TYR:OH	2.13	0.48
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.95	0.48
1:P:349:PRO:HB2	1:P:351:VAL:HG22	1.94	0.48
1:P:442:LEU:O	1:P:443:GLY:C	2.56	0.48
1:P:190:GLN:HA	1:P:191:PRO:HA	1.63	0.48
1:P:318:TRP:HB2	1:P:322:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:266:GLY:O	1:P:267:ASP:C	2.57	0.47
1:P:136:PRO:HG2	1:P:144:PHE:CE2	2.49	0.47
1:P:197:LEU:O	1:P:198:GLU:C	2.56	0.47
1:P:145:LEU:HD12	1:P:182:LEU:O	2.15	0.47
1:P:279:THR:CG2	1:P:313:PRO:O	2.63	0.47
1:P:128:VAL:HB	4:P:2041:HOH:O	2.15	0.46
1:P:327:THR:CG2	4:P:2110:HOH:O	2.63	0.46
1:P:428:LEU:H	1:P:440:ASN:ND2	2.13	0.46
1:P:396:ALA:HB2	1:P:459:LEU:HD13	1.97	0.46
1:P:261:LEU:O	1:P:265:ILE:HG13	2.14	0.46
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.97	0.46
1:P:183:ALA:O	1:P:184:ASN:C	2.59	0.45
1:P:123:LYS:HD2	1:P:150:SER:HA	1.97	0.45
1:P:143:ARG:HD3	2:A:1:NAG:H82	1.97	0.45
1:P:70:THR:N	1:P:71:PRO:HD2	2.30	0.45
1:P:124:TRP:O	1:P:125:HIS:C	2.59	0.45
1:P:43:SER:OG	1:P:244:ARG:HG3	2.17	0.45
1:P:400:THR:HB	1:P:423:HIS:CE1	2.52	0.45
1:P:268:LEU:HB2	1:P:270:LEU:HG	1.99	0.45
1:P:440:ASN:ND2	1:P:442:LEU:H	2.14	0.45
1:P:202:MET:HE2	1:P:202:MET:CA	2.46	0.45
1:P:179:ILE:O	1:P:191:PRO:HA	2.17	0.44
1:P:81:LEU:HA	1:P:82:PRO:HD3	1.82	0.44
1:P:442:LEU:HD12	1:P:442:LEU:HA	1.82	0.43
1:P:198:GLU:O	1:P:201:TYR:N	2.52	0.43
1:P:318:TRP:CD2	1:P:321:HIS:HB2	2.54	0.43
1:P:190:GLN:HG2	1:P:501:HIS:HA	2.01	0.43
1:P:500:CYS:O	1:P:501:HIS:CB	2.62	0.43
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.54	0.42
1:P:24:VAL:HG13	1:P:276:VAL:HG22	2.01	0.42
1:P:227:HIS:HA	4:P:2072:HOH:O	2.18	0.42
1:P:348:LEU:O	1:P:349:PRO:C	2.61	0.42
1:P:198:GLU:HG3	4:P:2069:HOH:O	2.15	0.42
1:P:28:ALA:HB2	1:P:254:LEU:HD11	2.02	0.41
1:P:112:ALA:O	1:P:115:GLY:N	2.47	0.41
1:P:177:VAL:HG22	1:P:500:CYS:HB2	2.03	0.41
1:P:278:PHE:O	1:P:314:ALA:HA	2.21	0.41
1:P:23:ILE:HD13	1:P:340:LEU:HD22	2.03	0.40
1:P:213:GLN:O	1:P:216:ASP:N	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	476/489 (97%)	440 (92%)	32 (7%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS
1	P	502	CYS
1	P	172	CYS
1	P	501	HIS

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	370/384 (96%)	325 (88%)	45 (12%)	5	10

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	52	LEU
1	P	85	MET
1	P	96	SER
1	P	103	GLU
1	P	111	LEU
1	P	161	CYS
1	P	169	ASP

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Mol	Chain	Res	Type
1	P	177	VAL
1	P	179	ILE
1	P	185	LEU
1	P	188	GLU
1	P	197	LEU
1	P	215	GLU
1	P	236	GLN
1	P	237	SER
1	P	240	GLU
1	P	254	LEU
1	P	261	LEU
1	P	262	MET
1	P	272	GLU
1	P	279	THR
1	P	282	ASN
1	P	327	THR
1	P	334	LEU
1	P	336	LEU
1	P	337	LEU
1	P	343	LEU
1	P	351	VAL
1	P	352	THR
1	P	362	LEU
1	P	363	LEU
1	P	367	LYS
1	P	368	SER
1	P	377	PRO
1	P	400	THR
1	P	426	LEU
1	P	442	LEU
1	P	449	THR
1	P	451	GLU
1	P	453	LEU
1	P	456	LEU
1	P	470	VAL
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	48	ASN
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
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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	DDZ	P	69	3,1	4,6,7	1.26	1 (25%)	3,7,9	2.66	2 (66%)

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
1	DDZ	P	69	3,1	-	0/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	69	DDZ	OG2-CB	2.05	1.44	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	69	DDZ	OG2-CB-OG1	3.88	117.96	111.26
1	P	69	DDZ	O-C-CA	-2.28	118.92	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	2.15	5 (35%)	17,19,21	3.96	11 (64%)
2	NAG	A	2	2	14,14,15	1.45	3 (21%)	17,19,21	2.67	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	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	2	2	1/1/5/7	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	C2-N2	4.68	1.54	1.46
2	A	2	NAG	O7-C7	-3.60	1.15	1.23
2	A	1	NAG	O7-C7	-3.46	1.15	1.23
2	A	1	NAG	O4-C4	-3.05	1.35	1.43
2	A	1	NAG	O5-C5	-2.88	1.37	1.43
2	A	2	NAG	C1-C2	2.43	1.55	1.52
2	A	1	NAG	C4-C5	2.18	1.57	1.53
2	A	2	NAG	C2-N2	2.14	1.49	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	C1-O5-C5	9.17	124.48	112.19
2	A	1	NAG	C8-C7-N2	7.72	128.91	116.12
2	A	1	NAG	O7-C7-N2	-6.55	110.41	121.98
2	A	1	NAG	O4-C4-C3	6.35	125.34	110.38
2	A	1	NAG	C1-O5-C5	5.43	119.46	112.19
2	A	1	NAG	O4-C4-C5	-4.67	97.82	109.32
2	A	1	NAG	C2-N2-C7	-4.17	117.31	122.90
2	A	1	NAG	C3-C4-C5	-3.94	103.08	110.23
2	A	1	NAG	C6-C5-C4	-3.07	105.49	113.02
2	A	1	NAG	O5-C1-C2	2.96	115.88	111.29
2	A	2	NAG	O3-C3-C2	-2.91	103.36	109.40
2	A	1	NAG	O5-C5-C6	2.83	113.18	107.66
2	A	2	NAG	C2-N2-C7	-2.40	119.68	122.90
2	A	1	NAG	C4-C3-C2	2.26	114.33	111.02
2	A	2	NAG	O5-C1-C2	-2.24	107.82	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:

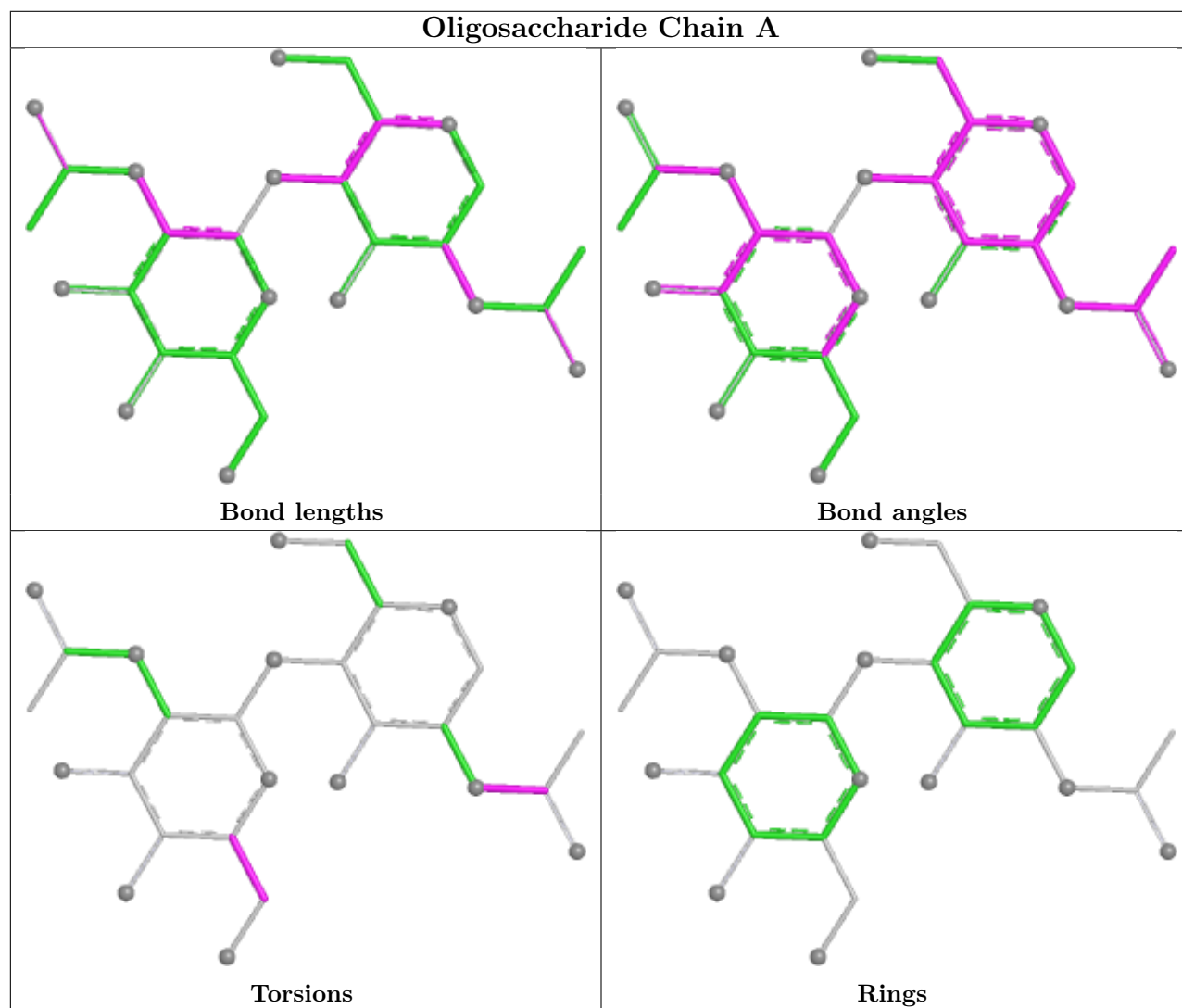
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	A	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	NAG	2	0
2	A	1	NAG	3	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 ⓘ

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

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, 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	480/489 (98%)	-0.33	8 (1%) 69 65	18, 38, 64, 92	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	448	ALA	4.2
1	P	443	GLY	2.8
1	P	503	PRO	2.6
1	P	19	ARG	2.4
1	P	490	HIS	2.4
1	P	131	GLU	2.2
1	P	501	HIS	2.1
1	P	350	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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.

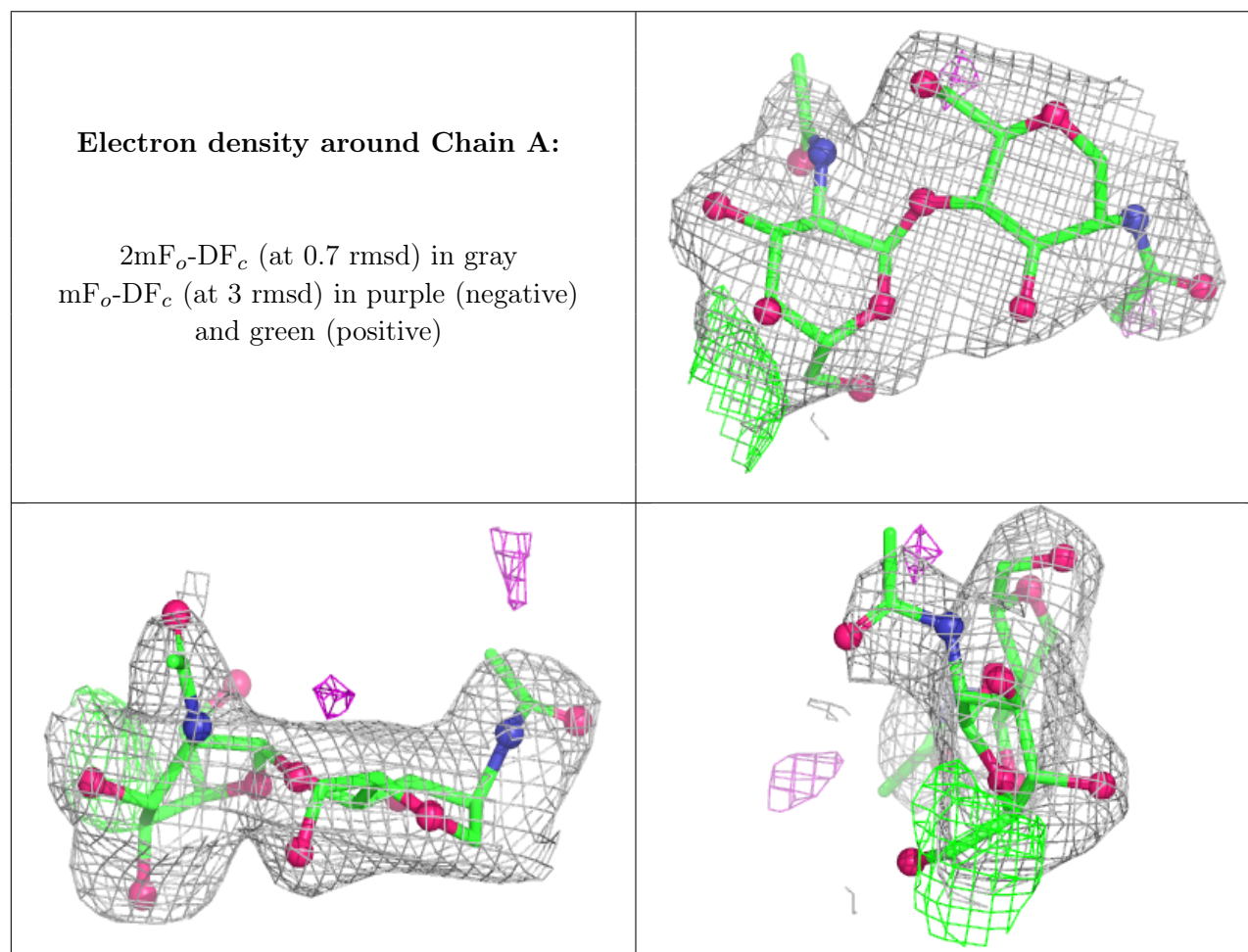
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	DDZ	P	69	7/8	0.92	0.07	28,28,32,33	0

6.3 Carbohydrates

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($\text{\AA}^2$)	Q<0.9
2	NAG	A	1	14/15	-	-	54,60,72,80	0
2	NAG	A	2	14/15	-	-	86,94,107,111	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 ⓘ

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($\text{\AA}^2$)	Q<0.9
3	MG	P	603	1/1	0.98	0.10	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.