



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 AM UTC

PDB ID : 1E3C / pdb_00001e3c
Title : Crystal structure of an Arylsulfatase A mutant C69S soaked in synthetic substrate
Authors : von Buelow, R.; Schmidt, B.; Dierks, T.; von Figura, K.; Uson, I.
Deposited on : 2000-06-13
Resolution : 2.65 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

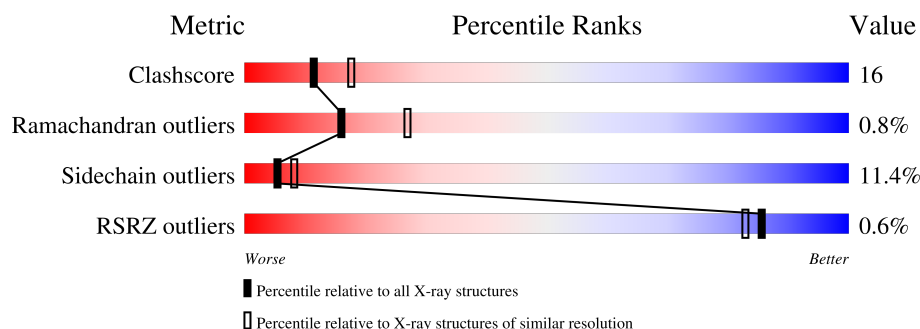
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	40% 41% 15% ...
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

There are 4 unique types of molecules in this entry. The entry contains 3784 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
			3582	2282	610	667	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	69	SER	CYS	engineered mutation	UNP P15289
P	215	GLU	GLN	conflict	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		

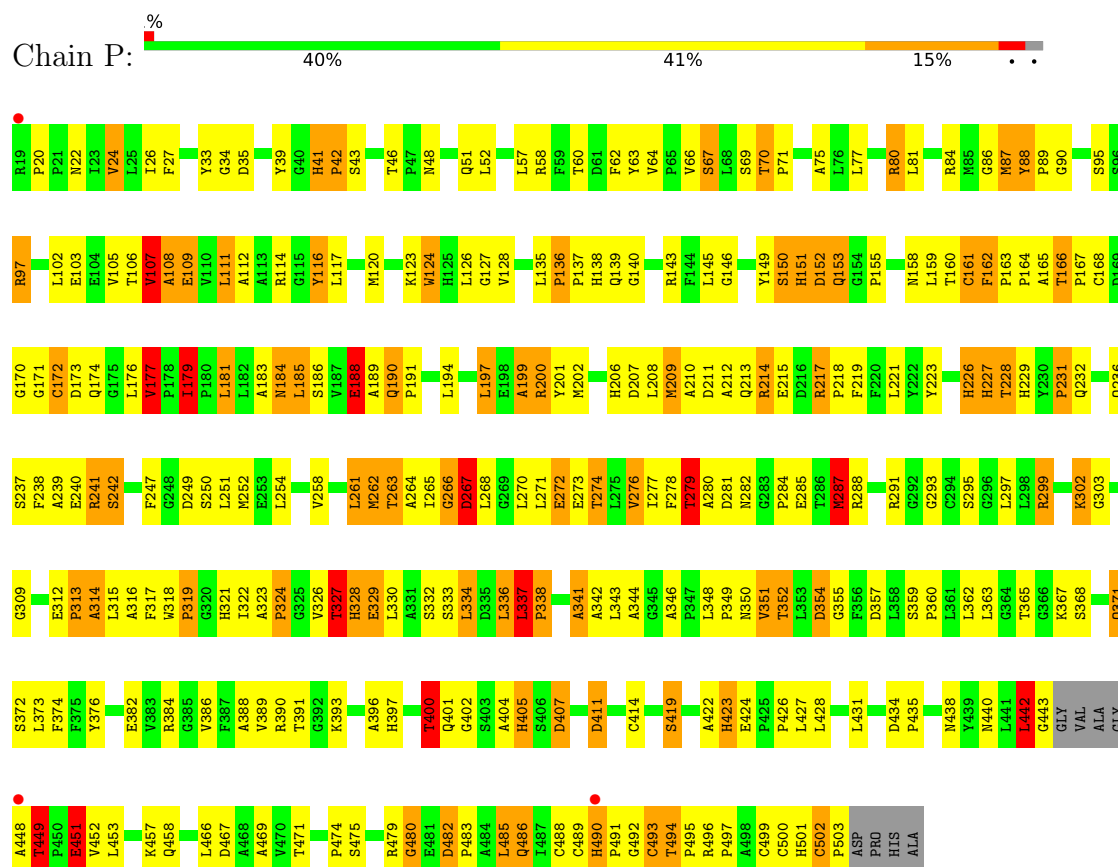
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	173	Total	O	0	0
			173	173		

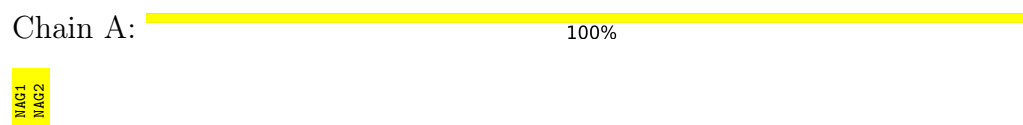
3 Residue-property plots

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 – 2.65 40.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.65) 99.3 (40.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.64Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.243 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 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	3784	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	1.29	8/3689 (0.2%)	2.65	338/5042 (6.7%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	490	HIS	N-CA	-9.06	1.36	1.46
1	P	502	CYS	C-O	-8.46	1.14	1.24
1	P	503	PRO	N-CD	7.27	1.57	1.47
1	P	151	HIS	CE1-NE2	5.50	1.38	1.32
1	P	242	SER	C-O	5.28	1.30	1.23
1	P	43	SER	C-O	-5.25	1.17	1.24
1	P	424	GLU	C-O	-5.14	1.21	1.25
1	P	285	GLU	CA-CB	-5.06	1.46	1.52

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	489	CYS	CA-C-N	17.90	146.43	123.34
1	P	489	CYS	C-N-CA	17.90	146.43	123.34
1	P	179	ILE	CA-CB-CG2	13.73	133.85	110.50
1	P	496	ARG	CA-C-O	-13.00	106.97	120.23
1	P	494	THR	CA-C-O	-12.53	107.13	119.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	424	GLU	CA-C-O	-12.24	106.88	119.49
1	P	338	PRO	O-C-N	-12.11	108.32	122.24
1	P	291	ARG	NE-CZ-NH2	-11.87	108.52	119.20
1	P	171	GLY	N-CA-C	11.47	130.54	115.40
1	P	327	THR	CB-CA-C	-11.41	90.22	109.50
1	P	190	GLN	OE1-CD-NE2	-10.94	111.66	122.60
1	P	177	VAL	N-CA-CB	-10.93	96.88	110.33
1	P	494	THR	O-C-N	10.70	129.34	121.85
1	P	404	ALA	CA-C-O	-10.56	109.35	120.55
1	P	352	THR	CA-C-O	10.52	132.91	120.81
1	P	502	CYS	N-CA-CB	-10.11	97.31	111.77
1	P	190	GLN	CB-CG-CD	9.51	128.78	112.60
1	P	35	ASP	CA-C-O	-9.43	109.78	120.24
1	P	114	ARG	CA-C-O	9.39	130.56	119.48
1	P	384	ARG	CD-NE-CZ	-9.04	111.75	124.40
1	P	209	MET	CA-C-N	8.98	133.28	120.79
1	P	209	MET	C-N-CA	8.98	133.28	120.79
1	P	217	ARG	NE-CZ-NH2	8.98	127.28	119.20
1	P	350	ASN	CA-CB-CG	-8.98	103.62	112.60
1	P	177	VAL	CB-CA-C	8.96	119.67	110.88
1	P	267	ASP	CA-CB-CG	-8.94	103.66	112.60
1	P	155	PRO	CA-C-O	-8.92	111.17	121.34
1	P	188	GLU	O-C-N	-8.86	111.38	122.27
1	P	267	ASP	CA-C-O	-8.78	107.96	120.51
1	P	279	THR	CB-CA-C	-8.69	95.76	114.10
1	P	127	GLY	CA-C-O	8.67	127.85	122.22
1	P	449	THR	CA-CB-OG1	-8.65	96.63	109.60
1	P	27	PHE	CA-CB-CG	8.60	122.40	113.80
1	P	411	ASP	CA-C-O	8.51	125.62	119.32
1	P	423	HIS	CA-CB-CG	-8.51	105.29	113.80
1	P	368	SER	CA-C-O	8.44	128.24	119.80
1	P	160	THR	CA-CB-OG1	-8.42	96.97	109.60
1	P	200	ARG	NE-CZ-NH2	8.32	126.69	119.20
1	P	219	PHE	O-C-N	-8.31	113.64	123.03
1	P	63	TYR	N-CA-C	8.20	122.23	109.52
1	P	249	ASP	CA-C-O	8.09	129.13	120.55
1	P	391	THR	OG1-CB-CG2	-8.09	93.12	109.30
1	P	479	ARG	CD-NE-CZ	8.09	135.72	124.40
1	P	190	GLN	CG-CD-NE2	8.08	128.52	116.40
1	P	435	PRO	CA-C-N	8.07	134.62	120.74
1	P	435	PRO	C-N-CA	8.07	134.62	120.74
1	P	120	MET	CG-SD-CE	-8.02	83.25	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	263	THR	O-C-N	-8.02	113.81	122.07
1	P	319	PRO	CA-C-O	7.96	130.42	121.34
1	P	404	ALA	O-C-N	7.86	130.46	122.12
1	P	382	GLU	CA-C-O	-7.80	109.63	119.31
1	P	238	PHE	CA-CB-CG	-7.78	106.02	113.80
1	P	242	SER	CA-C-N	-7.74	106.25	121.41
1	P	242	SER	C-N-CA	-7.74	106.25	121.41
1	P	138	HIS	CA-CB-CG	-7.71	106.09	113.80
1	P	114	ARG	N-CA-C	-7.66	102.14	112.94
1	P	22	ASN	OD1-CG-ND2	7.64	130.24	122.60
1	P	279	THR	N-CA-CB	7.58	122.82	110.55
1	P	448	ALA	O-C-N	-7.54	110.94	123.00
1	P	186	SER	O-C-N	7.51	132.99	123.23
1	P	174	GLN	CG-CD-NE2	7.50	127.66	116.40
1	P	176	LEU	CA-C-O	7.50	130.24	121.46
1	P	326	VAL	CA-C-O	-7.44	111.48	120.78
1	P	140	GLY	CA-C-N	-7.43	111.72	122.19
1	P	140	GLY	C-N-CA	-7.43	111.72	122.19
1	P	120	MET	CA-C-O	-7.39	111.19	120.28
1	P	219	PHE	CA-C-N	7.34	134.00	123.14
1	P	219	PHE	C-N-CA	7.34	134.00	123.14
1	P	302	LYS	CA-C-N	-7.32	112.18	122.86
1	P	302	LYS	C-N-CA	-7.32	112.18	122.86
1	P	186	SER	CA-C-O	-7.30	112.81	120.70
1	P	184	ASN	CA-CB-CG	-7.28	105.32	112.60
1	P	107	VAL	N-CA-CB	7.28	120.44	110.54
1	P	279	THR	CA-CB-OG1	7.27	120.51	109.60
1	P	352	THR	O-C-N	-7.26	114.00	122.93
1	P	291	ARG	NH1-CZ-NH2	7.25	128.72	119.30
1	P	488	CYS	CA-C-N	7.24	135.36	121.54
1	P	488	CYS	C-N-CA	7.24	135.36	121.54
1	P	287	MET	O-C-N	-7.15	114.05	122.20
1	P	475	SER	N-CA-CB	-7.13	98.78	109.69
1	P	66	VAL	O-C-N	-7.13	115.37	123.07
1	P	271	LEU	N-CA-CB	7.12	122.53	110.49
1	P	438	ASN	OD1-CG-ND2	7.12	129.72	122.60
1	P	277	ILE	CA-C-O	-7.09	112.97	120.48
1	P	448	ALA	CA-C-O	7.03	132.75	120.80
1	P	139	GLN	CG-CD-NE2	6.97	126.85	116.40
1	P	354	ASP	CA-CB-CG	6.96	119.56	112.60
1	P	247	PHE	CA-CB-CG	-6.95	106.85	113.80
1	P	438	ASN	CA-CB-CG	-6.95	105.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	467	ASP	O-C-N	-6.92	114.78	122.12
1	P	355	GLY	O-C-N	-6.91	117.58	123.59
1	P	407	ASP	CA-CB-CG	6.90	119.50	112.60
1	P	67	SER	CA-CB-OG	-6.88	97.34	111.10
1	P	354	ASP	CB-CG-OD1	6.86	134.17	118.40
1	P	400	THR	N-CA-CB	-6.85	98.79	111.53
1	P	20	PRO	O-C-N	6.84	129.54	121.46
1	P	152	ASP	CA-C-N	-6.84	111.81	122.08
1	P	152	ASP	C-N-CA	-6.84	111.81	122.08
1	P	232	GLN	CA-C-N	6.82	133.55	121.75
1	P	232	GLN	C-N-CA	6.82	133.55	121.75
1	P	162	PHE	CA-CB-CG	-6.80	107.00	113.80
1	P	274	THR	N-CA-C	6.79	119.97	108.90
1	P	327	THR	OG1-CB-CG2	6.72	122.74	109.30
1	P	496	ARG	CA-CB-CG	6.67	127.44	114.10
1	P	189	ALA	CA-C-O	-6.67	113.77	121.10
1	P	64	VAL	O-C-N	-6.65	113.52	121.10
1	P	69	SER	N-CA-C	6.62	118.16	111.07
1	P	336	LEU	N-CA-C	6.62	119.34	111.33
1	P	80	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	P	474	PRO	N-CA-CB	6.61	109.19	103.31
1	P	489	CYS	CA-CB-SG	-6.60	99.21	114.40
1	P	217	ARG	CD-NE-CZ	-6.59	115.17	124.40
1	P	401	GLN	N-CA-CB	-6.56	99.41	110.49
1	P	497	PRO	CA-N-CD	-6.55	102.33	111.50
1	P	87	MET	CA-C-N	6.54	131.54	122.06
1	P	87	MET	C-N-CA	6.54	131.54	122.06
1	P	391	THR	N-CA-CB	6.53	121.02	110.77
1	P	221	LEU	CA-C-N	6.52	132.42	122.77
1	P	221	LEU	C-N-CA	6.52	132.42	122.77
1	P	384	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	P	371	GLN	CA-C-N	6.49	132.74	122.62
1	P	371	GLN	C-N-CA	6.49	132.74	122.62
1	P	471	THR	N-CA-CB	6.48	121.21	110.52
1	P	352	THR	CB-CA-C	6.46	120.23	109.89
1	P	396	ALA	CA-C-N	-6.42	114.22	122.77
1	P	396	ALA	C-N-CA	-6.42	114.22	122.77
1	P	124	TRP	CA-C-N	6.42	131.71	122.40
1	P	124	TRP	C-N-CA	6.42	131.71	122.40
1	P	346	ALA	N-CA-C	-6.42	101.99	110.40
1	P	107	VAL	O-C-N	6.40	128.08	121.87
1	P	185	LEU	CA-C-N	-6.39	113.36	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	185	LEU	C-N-CA	-6.39	113.36	122.94
1	P	333	SER	O-C-N	-6.36	114.12	122.39
1	P	453	LEU	N-CA-CB	-6.33	100.48	110.22
1	P	51	GLN	CB-CG-CD	-6.31	101.87	112.60
1	P	88	TYR	CB-CA-C	-6.28	103.09	110.76
1	P	106	THR	CA-C-O	-6.26	114.24	121.82
1	P	299	ARG	NH1-CZ-NH2	6.25	127.43	119.30
1	P	299	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	P	344	ALA	CA-C-O	6.21	126.92	119.59
1	P	158	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	P	106	THR	O-C-N	6.20	129.89	122.20
1	P	184	ASN	CA-C-O	-6.19	111.65	120.51
1	P	327	THR	CA-C-N	6.18	132.25	122.60
1	P	327	THR	C-N-CA	6.18	132.25	122.60
1	P	480	GLY	CA-C-O	-6.18	116.89	122.57
1	P	299	ARG	N-CA-CB	-6.18	100.22	110.23
1	P	51	GLN	CA-C-O	-6.17	113.88	120.42
1	P	199	ALA	N-CA-CB	-6.14	101.10	110.01
1	P	402	GLY	N-CA-C	-6.13	103.21	112.41
1	P	189	ALA	O-C-N	6.11	129.51	123.46
1	P	329	GLU	CA-C-N	-6.08	112.23	120.87
1	P	329	GLU	C-N-CA	-6.08	112.23	120.87
1	P	341	ALA	O-C-N	-6.08	114.50	122.59
1	P	184	ASN	OD1-CG-ND2	6.06	128.66	122.60
1	P	323	ALA	N-CA-CB	-6.05	101.61	110.14
1	P	86	GLY	CA-C-O	-6.04	111.52	119.25
1	P	400	THR	CA-CB-CG2	6.04	120.77	110.50
1	P	226	HIS	CA-CB-CG	-6.03	107.77	113.80
1	P	314	ALA	CB-CA-C	6.02	120.06	109.89
1	P	135	LEU	CA-C-O	-6.02	114.25	120.87
1	P	278	PHE	CA-CB-CG	6.01	119.81	113.80
1	P	453	LEU	O-C-N	-6.01	115.18	122.22
1	P	112	ALA	N-CA-C	-6.00	104.82	111.36
1	P	354	ASP	OD1-CG-OD2	-5.99	108.52	122.90
1	P	273	GLU	CA-C-O	5.99	126.25	119.18
1	P	116	TYR	O-C-N	-5.97	116.23	123.16
1	P	242	SER	CA-C-O	-5.97	114.77	121.81
1	P	262	MET	N-CA-C	-5.97	104.85	111.36
1	P	263	THR	CA-C-O	5.97	127.09	120.82
1	P	391	THR	CA-C-O	5.95	126.55	120.24
1	P	434	ASP	CA-C-N	5.92	125.79	119.28
1	P	434	ASP	C-N-CA	5.92	125.79	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	179	ILE	N-CA-CB	-5.90	102.95	111.21
1	P	136	PRO	N-CA-C	5.88	117.87	110.70
1	P	41	HIS	CB-CA-C	5.87	118.84	109.62
1	P	188	GLU	CB-CG-CD	-5.87	102.62	112.60
1	P	315	LEU	O-C-N	-5.86	116.32	123.30
1	P	372	SER	CA-CB-OG	-5.86	99.38	111.10
1	P	384	ARG	NH1-CZ-NH2	5.85	126.91	119.30
1	P	333	SER	CA-C-O	5.84	126.56	119.49
1	P	303	GLY	CA-C-O	-5.84	113.02	119.27
1	P	165	ALA	N-CA-CB	-5.84	101.21	111.42
1	P	329	GLU	CB-CG-CD	-5.81	102.72	112.60
1	P	152	ASP	N-CA-C	-5.77	105.90	113.17
1	P	108	ALA	O-C-N	-5.76	116.13	122.07
1	P	67	SER	N-CA-CB	-5.75	100.77	110.49
1	P	496	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	P	135	LEU	CA-C-N	5.75	126.30	120.38
1	P	135	LEU	C-N-CA	5.75	126.30	120.38
1	P	389	VAL	CA-C-O	-5.74	114.45	120.76
1	P	153	GLN	CA-C-N	5.74	130.87	121.87
1	P	153	GLN	C-N-CA	5.74	130.87	121.87
1	P	272	GLU	CA-C-O	-5.73	112.32	120.51
1	P	295	SER	N-CA-C	-5.72	105.88	112.92
1	P	184	ASN	CA-C-N	-5.72	114.11	122.86
1	P	184	ASN	C-N-CA	-5.72	114.11	122.86
1	P	482	ASP	CA-C-N	5.72	125.57	119.28
1	P	482	ASP	C-N-CA	5.72	125.57	119.28
1	P	295	SER	CA-CB-OG	-5.71	99.68	111.10
1	P	146	GLY	N-CA-C	5.69	118.26	110.69
1	P	218	PRO	CA-C-N	-5.69	112.38	122.74
1	P	218	PRO	C-N-CA	-5.69	112.38	122.74
1	P	197	LEU	N-CA-CB	-5.69	101.53	110.06
1	P	422	ALA	O-C-N	-5.68	116.54	122.96
1	P	368	SER	O-C-N	-5.67	115.61	121.28
1	P	438	ASN	CB-CA-C	-5.65	98.32	109.67
1	P	281	ASP	CB-CG-OD1	5.64	131.38	118.40
1	P	80	ARG	NE-CZ-NH1	-5.63	115.86	121.50
1	P	181	LEU	CA-C-O	-5.63	114.13	120.43
1	P	330	LEU	O-C-N	-5.62	116.04	122.89
1	P	227	HIS	N-CA-CB	-5.61	101.72	109.97
1	P	495	PRO	N-CD-CG	5.60	110.52	103.80
1	P	360	PRO	O-C-N	5.60	128.95	122.23
1	P	109	GLU	CA-CB-CG	-5.59	102.91	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	200	ARG	CA-C-N	-5.59	111.81	120.31
1	P	200	ARG	C-N-CA	-5.59	111.81	120.31
1	P	326	VAL	O-C-N	-5.59	115.58	122.57
1	P	41	HIS	O-C-N	-5.58	116.33	121.30
1	P	280	ALA	CA-C-O	-5.57	114.75	120.99
1	P	139	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	P	486	GLN	CA-C-N	5.55	128.80	120.69
1	P	486	GLN	C-N-CA	5.55	128.80	120.69
1	P	39	TYR	N-CA-C	-5.55	105.12	112.94
1	P	442	LEU	O-C-N	-5.52	115.25	122.59
1	P	363	LEU	CD1-CG-CD2	5.52	122.94	110.80
1	P	97	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	P	207	ASP	CA-CB-CG	5.51	118.11	112.60
1	P	503	PRO	CA-N-CD	-5.51	104.28	112.00
1	P	337	LEU	CA-C-O	5.50	124.31	119.08
1	P	39	TYR	N-CA-CB	5.50	120.05	110.98
1	P	499	CYS	CA-C-N	-5.49	112.74	122.07
1	P	499	CYS	C-N-CA	-5.49	112.74	122.07
1	P	247	PHE	CA-C-O	5.48	126.23	120.42
1	P	453	LEU	CA-C-O	5.48	126.29	120.10
1	P	303	GLY	N-CA-C	-5.46	108.19	114.69
1	P	291	ARG	CD-NE-CZ	5.45	132.04	124.40
1	P	143	ARG	NE-CZ-NH2	-5.45	114.30	119.20
1	P	166	THR	CA-C-O	5.45	127.63	120.16
1	P	327	THR	CA-CB-OG1	-5.45	101.42	109.60
1	P	312	GLU	CB-CG-CD	-5.45	103.34	112.60
1	P	309	GLY	CA-C-O	-5.45	111.09	120.57
1	P	90	GLY	O-C-N	-5.44	115.62	122.70
1	P	405	HIS	ND1-CE1-NE2	5.44	113.84	108.40
1	P	223	TYR	O-C-N	-5.44	116.00	122.63
1	P	214	ARG	CA-C-O	-5.43	112.92	119.49
1	P	228	THR	CA-C-O	5.43	130.03	120.80
1	P	107	VAL	CB-CA-C	-5.42	104.82	112.14
1	P	226	HIS	N-CA-CB	5.42	118.46	110.33
1	P	332	SER	N-CA-C	5.41	117.91	109.52
1	P	26	ILE	CB-CA-C	-5.41	104.20	110.91
1	P	469	ALA	N-CA-C	5.41	119.97	112.45
1	P	173	ASP	O-C-N	-5.39	116.73	123.04
1	P	48	ASN	CB-CG-ND2	5.37	124.45	116.40
1	P	497	PRO	N-CD-CG	5.37	110.25	103.80
1	P	150	SER	CB-CA-C	5.36	118.38	109.53
1	P	351	VAL	O-C-N	5.36	128.99	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	502	CYS	CB-CA-C	5.36	117.61	110.81
1	P	424	GLU	O-C-N	5.35	128.90	121.47
1	P	323	ALA	CA-C-O	5.34	125.68	120.23
1	P	449	THR	N-CA-CB	-5.34	100.87	110.37
1	P	231	PRO	CB-CA-C	-5.32	98.69	112.00
1	P	95	SER	CA-C-O	5.32	125.86	119.43
1	P	351	VAL	CB-CA-C	-5.31	102.48	110.55
1	P	173	ASP	CA-C-O	5.30	126.74	120.69
1	P	229	HIS	O-C-N	-5.30	116.97	122.96
1	P	495	PRO	CA-N-CD	-5.29	104.09	111.50
1	P	374	PHE	CA-C-O	-5.28	114.62	120.38
1	P	426	PRO	CA-C-N	5.27	128.32	120.95
1	P	426	PRO	C-N-CA	5.27	128.32	120.95
1	P	419	SER	N-CA-C	5.24	116.85	110.41
1	P	250	SER	N-CA-CB	-5.23	102.17	110.28
1	P	288	ARG	CG-CD-NE	-5.23	100.49	112.00
1	P	502	CYS	O-C-N	5.22	124.89	121.23
1	P	419	SER	O-C-N	-5.22	116.28	122.65
1	P	293	GLY	CA-C-N	5.22	131.09	122.33
1	P	293	GLY	C-N-CA	5.22	131.09	122.33
1	P	328	HIS	N-CA-C	-5.21	106.16	112.88
1	P	20	PRO	CA-C-O	-5.20	113.02	120.56
1	P	105	VAL	N-CA-CB	-5.20	104.91	111.46
1	P	57	LEU	N-CA-CB	-5.20	101.94	110.42
1	P	116	TYR	N-CA-CB	-5.20	101.81	110.23
1	P	373	LEU	CA-C-O	-5.20	114.68	120.66
1	P	302	LYS	N-CA-CB	-5.19	101.00	109.56
1	P	258	VAL	O-C-N	5.19	127.00	121.91
1	P	51	GLN	CA-CB-CG	5.19	124.47	114.10
1	P	42	PRO	CA-C-N	-5.18	114.05	121.98
1	P	42	PRO	C-N-CA	-5.18	114.05	121.98
1	P	168	CYS	CA-CB-SG	-5.17	102.52	114.40
1	P	284	PRO	N-CA-C	5.16	119.58	111.38
1	P	451	GLU	N-CA-C	-5.16	105.57	111.14
1	P	81	LEU	N-CA-C	-5.16	102.05	109.48
1	P	321	HIS	CA-CB-CG	-5.16	108.64	113.80
1	P	167	PRO	CA-C-O	-5.15	115.38	121.67
1	P	251	LEU	N-CA-C	-5.15	105.74	112.23
1	P	231	PRO	N-CA-CB	5.15	108.27	102.60
1	P	324	PRO	CB-CA-C	-5.15	103.06	111.56
1	P	210	ALA	CA-C-O	-5.15	115.41	121.07
1	P	503	PRO	N-CD-CG	-5.15	95.48	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	170	GLY	CA-C-N	-5.14	113.41	122.09
1	P	170	GLY	C-N-CA	-5.14	113.41	122.09
1	P	277	ILE	CB-CG1-CD1	-5.14	103.00	113.80
1	P	434	ASP	CA-CB-CG	5.14	117.74	112.60
1	P	143	ARG	CA-C-N	5.13	129.90	121.58
1	P	143	ARG	C-N-CA	5.13	129.90	121.58
1	P	217	ARG	CA-C-O	5.13	125.14	119.91
1	P	70	THR	N-CA-CB	5.12	117.49	110.11
1	P	288	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	P	414	CYS	N-CA-C	5.12	118.78	112.54
1	P	200	ARG	N-CA-C	-5.10	104.99	111.11
1	P	276	VAL	CB-CA-C	-5.10	103.52	110.96
1	P	206	HIS	CA-CB-CG	-5.09	108.70	113.80
1	P	483	PRO	N-CA-CB	5.09	108.89	103.39
1	P	344	ALA	O-C-N	-5.09	116.20	122.25
1	P	161	CYS	CB-CA-C	5.08	117.94	109.56
1	P	242	SER	N-CA-C	-5.08	103.70	110.55
1	P	435	PRO	CB-CA-C	-5.08	104.29	112.21
1	P	48	ASN	CA-CB-CG	-5.07	107.53	112.60
1	P	200	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	P	479	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	P	316	ALA	CA-C-O	5.06	125.60	120.24
1	P	33	TYR	CB-CG-CD2	-5.05	113.22	120.80
1	P	435	PRO	O-C-N	-5.05	115.70	122.22
1	P	239	ALA	CA-C-O	-5.04	114.90	120.70
1	P	388	ALA	O-C-N	-5.04	117.42	123.27
1	P	496	ARG	NH1-CZ-NH2	-5.04	112.74	119.30
1	P	48	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	P	458	GLN	CA-CB-CG	-5.03	104.04	114.10
1	P	239	ALA	N-CA-CB	5.03	117.45	109.51
1	P	354	ASP	O-C-N	-5.02	116.28	122.25
1	P	284	PRO	CB-CA-C	-5.02	104.41	110.98
1	P	367	LYS	CA-C-N	-5.02	113.95	120.67
1	P	367	LYS	C-N-CA	-5.02	113.95	120.67
1	P	46	THR	O-C-N	-5.01	116.99	121.20
1	P	313	PRO	CB-CA-C	-5.01	104.82	111.23
1	P	145	LEU	O-C-N	-5.01	116.51	123.12
1	P	474	PRO	O-C-N	5.01	129.09	123.03
1	P	58	ARG	CD-NE-CZ	-5.00	117.39	124.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	181	LEU	Mainchain
1	P	194	LEU	Mainchain
1	P	241	ARG	Mainchain
1	P	287	MET	Mainchain
1	P	42	PRO	Mainchain
1	P	442	LEU	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	3582	0	3454	114	1
2	A	28	0	25	0	0
3	P	1	0	0	0	0
4	P	173	0	0	20	1
All	All	3784	0	3479	114	2

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 (114) 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:2030:HOH:O	1.65	1.12
1:P:109:GLU:OE1	4:P:2034:HOH:O	1.90	0.88
1:P:423:HIS:HD2	4:P:2150:HOH:O	1.61	0.84
1:P:449:THR:HG22	1:P:451:GLU:H	1.53	0.74
1:P:442:LEU:O	1:P:443:GLY:C	2.30	0.73
1:P:24:VAL:HG13	1:P:276:VAL:HG22	1.71	0.73
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.72	0.70
1:P:357:ASP:OD2	4:P:2121:HOH:O	2.09	0.70
1:P:261:LEU:O	1:P:265:ILE:HG13	1.92	0.69
1:P:449:THR:HG22	1:P:451:GLU:N	2.06	0.68
1:P:163:PRO:HG2	1:P:236:GLN:HG3	1.77	0.66
1:P:393:LYS:NZ	4:P:2134:HOH:O	2.30	0.65
1:P:150:SER:H	1:P:153:GLN:NE2	1.95	0.64
1:P:150:SER:H	1:P:153:GLN:HE21	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:482:ASP:HB3	1:P:485:LEU:HD22	1.79	0.64
1:P:199:ALA:O	1:P:200:ARG:C	2.40	0.64
1:P:211:ASP:O	1:P:215:GLU:HG3	1.99	0.63
1:P:34:GLY:O	1:P:41:HIS:HB2	1.99	0.62
1:P:449:THR:CG2	1:P:451:GLU:H	2.12	0.61
1:P:84:ARG:HH11	1:P:84:ARG:HG2	1.66	0.61
1:P:357:ASP:OD1	1:P:359:SER:OG	2.17	0.59
1:P:263:THR:O	1:P:264:ALA:C	2.43	0.59
1:P:341:ALA:O	1:P:342:ALA:C	2.46	0.59
1:P:500:CYS:O	1:P:501:HIS:HB3	2.02	0.59
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.87	0.58
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.37	0.58
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.03	0.58
1:P:407:ASP:CB	4:P:2141:HOH:O	2.51	0.57
1:P:327:THR:HG23	4:P:2113:HOH:O	2.03	0.57
1:P:179:ILE:O	1:P:191:PRO:HA	2.05	0.57
1:P:318:TRP:HB2	1:P:322:ILE:HD12	1.87	0.56
1:P:242:SER:HB3	1:P:252:MET:HE2	1.88	0.56
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.87	0.56
1:P:400:THR:HG23	4:P:2147:HOH:O	2.06	0.55
1:P:209:MET:HE1	1:P:264:ALA:HB3	1.89	0.55
1:P:151:HIS:CD2	1:P:231:PRO:HD2	2.42	0.55
1:P:109:GLU:CD	4:P:2034:HOH:O	2.42	0.54
1:P:136:PRO:HB2	1:P:137:PRO:HD3	1.89	0.54
1:P:149:TYR:HE1	1:P:179:ILE:HD11	1.73	0.54
1:P:400:THR:HB	1:P:423:HIS:HE1	1.73	0.54
1:P:213:GLN:NE2	1:P:268:LEU:HB3	2.23	0.54
1:P:407:ASP:CG	4:P:2141:HOH:O	2.50	0.53
1:P:449:THR:HG22	1:P:452:VAL:H	1.72	0.53
1:P:390:ARG:HD2	1:P:431:LEU:HD12	1.90	0.53
1:P:150:SER:HB3	1:P:153:GLN:NE2	2.24	0.52
1:P:265:ILE:HD13	1:P:274:THR:HG21	1.91	0.52
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.92	0.52
1:P:348:LEU:O	1:P:349:PRO:C	2.52	0.51
1:P:109:GLU:OE2	4:P:2034:HOH:O	2.19	0.51
1:P:70:THR:N	1:P:71:PRO:HD2	2.26	0.50
1:P:241:ARG:CB	1:P:252:MET:HE1	2.42	0.50
1:P:159:LEU:HD21	1:P:191:PRO:HG3	1.94	0.50
1:P:70:THR:CG2	1:P:87:MET:HE3	2.42	0.50
1:P:337:LEU:HD12	1:P:338:PRO:N	2.27	0.49
1:P:400:THR:CG2	4:P:2147:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:299:ARG:HH21	1:P:411:ASP:CG	2.20	0.49
1:P:151:HIS:NE2	1:P:231:PRO:HD2	2.28	0.48
1:P:440:ASN:ND2	1:P:442:LEU:H	2.10	0.48
1:P:501:HIS:O	1:P:501:HIS:CG	2.67	0.48
1:P:327:THR:CG2	4:P:2113:HOH:O	2.61	0.48
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.26	0.48
1:P:268:LEU:O	1:P:270:LEU:HG	2.14	0.48
1:P:400:THR:HB	1:P:423:HIS:CE1	2.48	0.48
1:P:111:LEU:O	1:P:116:TYR:HB2	2.13	0.47
1:P:84:ARG:NH2	1:P:354:ASP:OD1	2.44	0.47
1:P:407:ASP:OD1	4:P:2141:HOH:O	2.20	0.47
1:P:197:LEU:HA	1:P:197:LEU:HD23	1.69	0.47
1:P:108:ALA:O	1:P:109:GLU:C	2.58	0.46
1:P:490:HIS:O	1:P:491:PRO:C	2.58	0.46
1:P:123:LYS:HD2	1:P:150:SER:HA	1.97	0.46
1:P:128:VAL:HB	4:P:2040:HOH:O	2.15	0.46
1:P:162:PHE:HB2	1:P:166:THR:HB	1.96	0.46
1:P:279:THR:CG2	1:P:313:PRO:O	2.64	0.46
1:P:428:LEU:H	1:P:440:ASN:ND2	2.14	0.46
1:P:190:GLN:HA	1:P:191:PRO:HA	1.73	0.45
1:P:266:GLY:O	1:P:267:ASP:C	2.57	0.45
1:P:327:THR:HG22	1:P:329:GLU:H	1.82	0.45
1:P:188:GLU:HG3	1:P:188:GLU:O	2.16	0.45
1:P:302:LYS:HD3	1:P:405:HIS:HB3	1.97	0.45
1:P:492:GLY:O	1:P:493:CYS:O	2.34	0.45
1:P:163:PRO:HA	1:P:164:PRO:C	2.42	0.45
1:P:152:ASP:HB3	1:P:231:PRO:HD3	1.98	0.45
1:P:337:LEU:HD12	1:P:337:LEU:C	2.41	0.45
1:P:329:GLU:OE2	4:P:2113:HOH:O	2.21	0.45
1:P:492:GLY:O	1:P:493:CYS:C	2.59	0.45
1:P:400:THR:CB	1:P:423:HIS:HE1	2.30	0.45
1:P:77:LEU:HD12	1:P:126:LEU:CD1	2.47	0.45
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.45	0.44
1:P:88:TYR:HB2	1:P:89:PRO:HA	1.99	0.44
1:P:183:ALA:O	1:P:184:ASN:C	2.58	0.44
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.52	0.44
1:P:318:TRP:CB	1:P:322:ILE:HD12	2.47	0.43
1:P:152:ASP:O	1:P:172:CYS:HB3	2.18	0.43
1:P:279:THR:HG22	1:P:313:PRO:O	2.19	0.43
1:P:149:TYR:HE1	1:P:179:ILE:CD1	2.31	0.43
1:P:123:LYS:NZ	1:P:150:SER:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:357:ASP:CG	4:P:2121:HOH:O	2.58	0.42
1:P:97:ARG:NH1	1:P:480:GLY:HA3	2.35	0.42
1:P:80:ARG:HG2	1:P:80:ARG:NH1	2.34	0.42
1:P:397:HIS:HB2	1:P:427:LEU:HB2	2.01	0.42
1:P:297:LEU:H	1:P:297:LEU:HD23	1.84	0.42
1:P:337:LEU:C	1:P:337:LEU:CD1	2.92	0.42
1:P:327:THR:CG2	1:P:329:GLU:H	2.33	0.42
1:P:423:HIS:CD2	4:P:2150:HOH:O	2.50	0.42
1:P:317:PHE:CE1	1:P:319:PRO:HD3	2.55	0.42
1:P:376:TYR:CZ	1:P:386:VAL:HG12	2.55	0.41
1:P:227:HIS:HA	1:P:228:THR:HA	1.79	0.41
1:P:502:CYS:O	1:P:502:CYS:SG	2.77	0.41
1:P:407:ASP:HB3	4:P:2141:HOH:O	2.19	0.41
1:P:202:MET:SD	1:P:261:LEU:CD1	3.09	0.41
1:P:329:GLU:OE1	4:P:2114:HOH:O	2.22	0.40
1:P:107:VAL:HG13	1:P:337:LEU:HB2	2.03	0.40
1:P:117:LEU:HD23	1:P:212:ALA:HB2	2.03	0.40
1:P:149:TYR:HB2	1:P:153:GLN:NE2	2.36	0.40

All (2) 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)
4:P:2148:HOH:O	4:P:2148:HOH:O[5_555]	1.84	0.36
1:P:490:HIS:NE2	1:P:490:HIS:NE2[16_554]	2.17	0.03

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%)	438 (92%)	35 (7%)	4 (1%)	16	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS
1	P	267	ASP
1	P	172	CYS
1	P	266	GLY

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	377/385 (98%)	334 (89%)	43 (11%)	5 8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	VAL
1	P	52	LEU
1	P	67	SER
1	P	103	GLU
1	P	107	VAL
1	P	111	LEU
1	P	161	CYS
1	P	177	VAL
1	P	179	ILE
1	P	185	LEU
1	P	188	GLU
1	P	208	LEU
1	P	214	ARG
1	P	217	ARG
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

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Mol	Chain	Res	Type
1	P	282	ASN
1	P	287	MET
1	P	324	PRO
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	365	THR
1	P	371	GLN
1	P	400	THR
1	P	419	SER
1	P	442	LEU
1	P	449	THR
1	P	451	GLU
1	P	457	LYS
1	P	466	LEU
1	P	485	LEU
1	P	494	THR

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	1,2	14,14,15	2.02	4 (28%)	17,19,21	3.58	10 (58%)
2	NAG	A	2	2	14,14,15	1.32	2 (14%)	17,19,21	2.56	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	1/1/5/7	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O7-C7	-4.28	1.13	1.23
2	A	1	NAG	C2-N2	4.21	1.53	1.46
2	A	2	NAG	O7-C7	-2.98	1.16	1.23
2	A	1	NAG	O5-C5	-2.72	1.38	1.43
2	A	1	NAG	O4-C4	-2.69	1.36	1.43
2	A	2	NAG	C2-N2	2.30	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C8-C7-N2	7.11	127.92	116.12
2	A	1	NAG	O7-C7-N2	-6.75	110.06	121.98
2	A	1	NAG	O4-C4-C3	5.25	122.75	110.38
2	A	2	NAG	C1-O5-C5	5.22	119.19	112.19
2	A	2	NAG	C2-N2-C7	-5.09	116.08	122.90
2	A	2	NAG	O3-C3-C2	-5.08	98.84	109.40
2	A	1	NAG	O5-C1-C2	4.45	118.18	111.29
2	A	1	NAG	O4-C4-C5	-4.21	98.96	109.32
2	A	1	NAG	C2-N2-C7	-3.67	117.98	122.90
2	A	2	NAG	C1-C2-N2	3.38	115.75	110.43
2	A	1	NAG	C1-O5-C5	3.31	116.62	112.19
2	A	1	NAG	C3-C4-C5	-3.13	104.56	110.23
2	A	1	NAG	O3-C3-C2	2.98	115.58	109.40
2	A	1	NAG	C6-C5-C4	-2.89	105.93	113.02
2	A	2	NAG	C3-C4-C5	2.15	114.13	110.23
2	A	2	NAG	C4-C3-C2	2.06	114.03	111.02

All (2) chirality outliers are listed below:

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

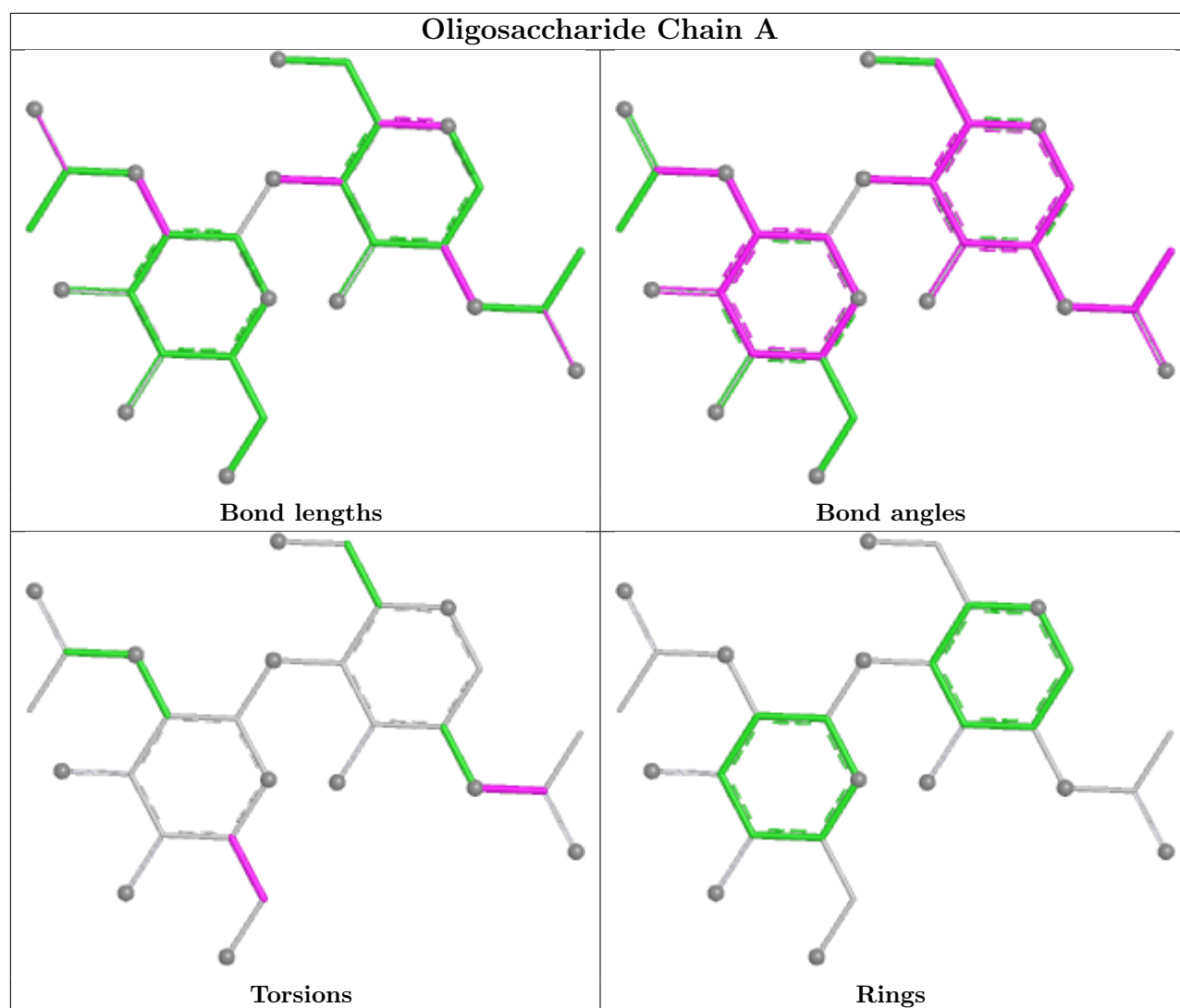
All (4) torsion outliers are listed below:

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.

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 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%)	-0.68	3 (0%) 85 83	15, 34, 61, 95	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	448	ALA	2.7
1	P	19	ARG	2.7
1	P	490	HIS	2.2

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

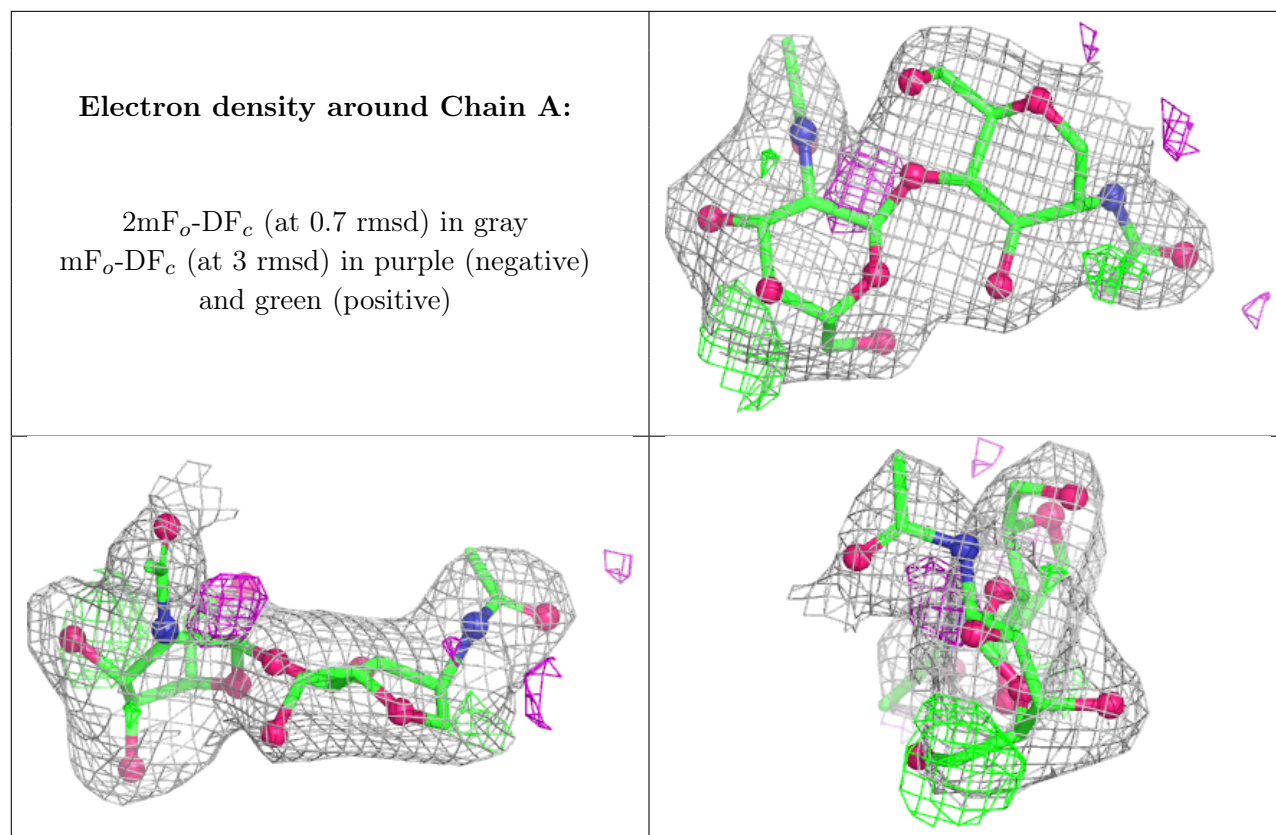
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	43,54,65,70	0
2	NAG	A	2	14/15	-	-	70,84,97,98	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
3	MG	P	603	1/1	0.96	0.07	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.