



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 5Z05 / pdb_00005z05
Title : Crystal structure of signalling protein from buffalo (SPB-40) with an acetone induced conformation of Trp78 at 1.49 Å resolution
Authors : Singh, P.K.; Chaudhary, A.; Tyagi, T.K.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2017-12-18
Resolution : 1.49 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

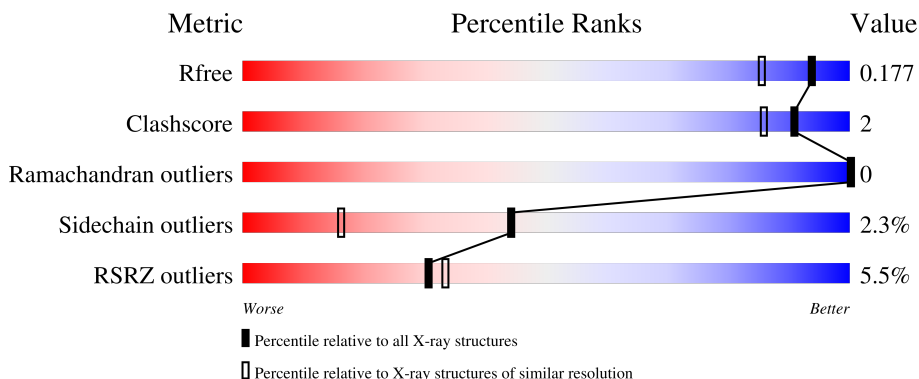
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

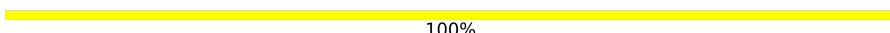
The reported resolution of this entry is 1.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	A	361	
2	B	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3336 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 Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	2	0
			2883	1846	499	529	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q7YS85

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



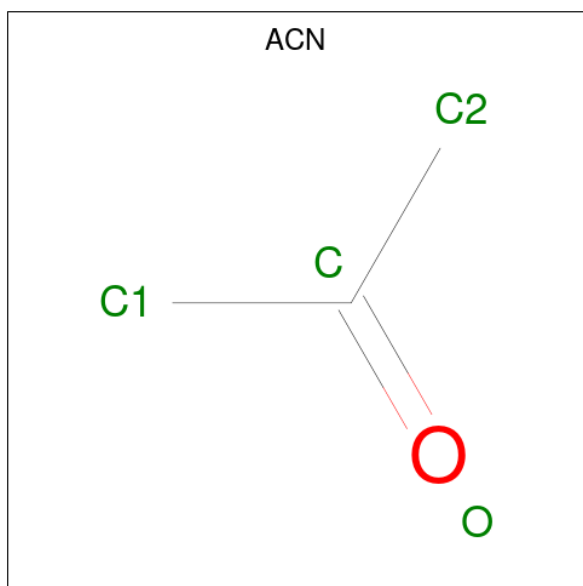
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is ACETONE (CCD ID: ACN) (formula: C_3H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		

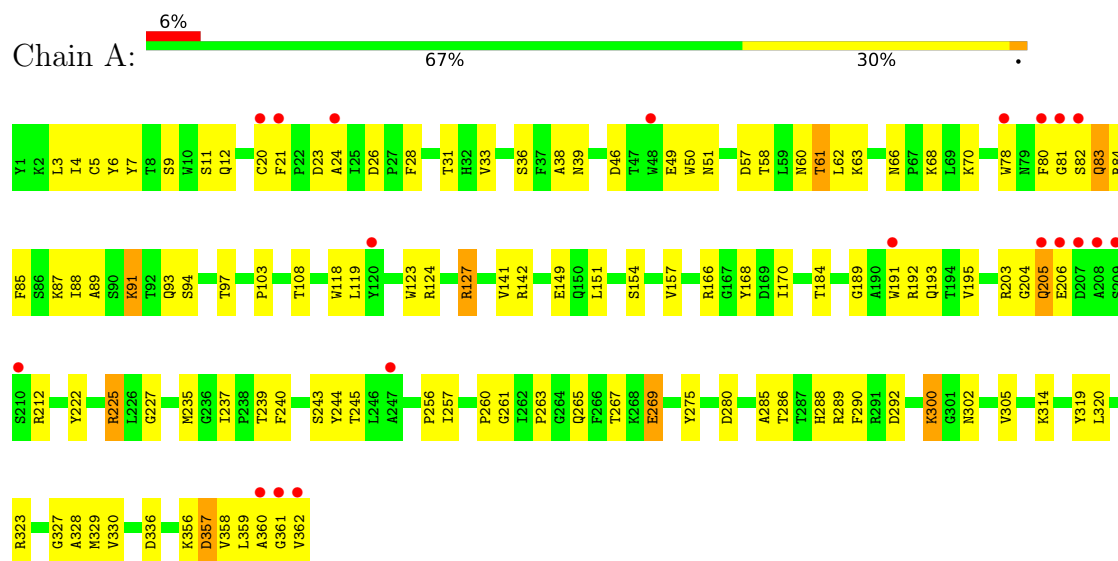
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	413	Total 413	O 413	0	0

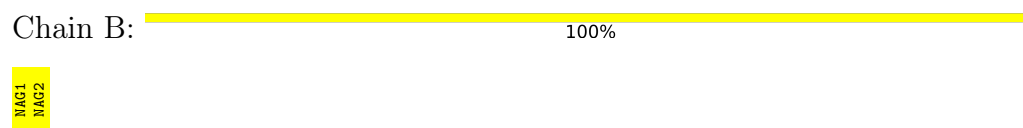
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chitinase-3-like protein 1



- 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.46Å 66.52Å 105.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.32 – 1.49 56.32 – 1.49	Depositor EDS
% Data completeness (in resolution range)	98.5 (56.32-1.49) 98.5 (56.32-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.147 , 0.176 0.148 , 0.177	Depositor DCC
R_{free} test set	3488 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3336	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: MPD, NAG, ACN

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	A	2.26	102/2972 (3.4%)	1.91	78/4031 (1.9%)

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	A	0	3

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	CYS	C-O	11.74	1.37	1.24
1	A	81	GLY	N-CA	10.42	1.60	1.45
1	A	118	TRP	C-O	-10.24	1.12	1.24
1	A	329	MET	SD-CE	-9.78	1.55	1.79
1	A	227	GLY	CA-C	-9.17	1.38	1.51
1	A	91	LYS	CE-NZ	-8.98	1.22	1.49
1	A	36	SER	CB-OG	-8.64	1.24	1.42
1	A	7	TYR	CZ-OH	8.47	1.55	1.38
1	A	300	LYS	N-CA	8.39	1.56	1.46
1	A	84	ARG	C-O	8.38	1.33	1.24
1	A	192	ARG	C-N	-8.03	1.21	1.33
1	A	193	GLN	N-CA	7.88	1.56	1.46
1	A	257	ILE	C-O	7.86	1.31	1.24
1	A	361	GLY	CA-C	7.82	1.63	1.52
1	A	89	ALA	CA-C	-7.77	1.41	1.52
1	A	261	GLY	N-CA	7.74	1.55	1.45
1	A	237	ILE	N-CA	7.60	1.51	1.45
1	A	9	SER	CA-CB	-7.59	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	ALA	C-O	7.52	1.33	1.24
1	A	61	THR	C-O	7.44	1.33	1.24
1	A	265	GLN	CD-OE1	7.35	1.37	1.23
1	A	11	SER	CA-C	-7.34	1.42	1.52
1	A	142	ARG	CD-NE	7.34	1.56	1.46
1	A	84	ARG	CZ-NH2	-7.32	1.24	1.33
1	A	119	LEU	C-O	7.24	1.33	1.23
1	A	85	PHE	N-CA	-7.17	1.37	1.46
1	A	123	TRP	N-CA	-7.10	1.37	1.46
1	A	108	THR	CA-CB	7.10	1.64	1.53
1	A	26	ASP	CA-C	7.05	1.61	1.52
1	A	154	SER	CA-C	-6.82	1.44	1.52
1	A	60	ASN	CG-ND2	6.75	1.47	1.33
1	A	330	VAL	C-O	6.74	1.31	1.24
1	A	260	PRO	C-O	-6.71	1.15	1.23
1	A	24	ALA	CA-C	6.69	1.61	1.52
1	A	195	VAL	C-O	6.68	1.32	1.24
1	A	118	TRP	C-N	-6.60	1.25	1.33
1	A	63	LYS	CD-CE	-6.50	1.32	1.52
1	A	142	ARG	NE-CZ	6.46	1.40	1.33
1	A	280	ASP	CB-CG	-6.43	1.35	1.52
1	A	23	ASP	CA-C	6.43	1.63	1.52
1	A	166	ARG	N-CA	6.39	1.54	1.46
1	A	280	ASP	N-CA	-6.39	1.38	1.46
1	A	151	LEU	CA-C	-6.37	1.44	1.52
1	A	21	PHE	N-CA	6.34	1.55	1.45
1	A	66	ASN	CA-C	6.33	1.59	1.52
1	A	225	ARG	NE-CZ	6.31	1.40	1.33
1	A	285	ALA	C-O	-6.30	1.15	1.23
1	A	327	GLY	CA-C	-6.29	1.44	1.52
1	A	94	SER	C-O	6.24	1.31	1.24
1	A	166	ARG	NE-CZ	6.16	1.39	1.33
1	A	222	TYR	CA-C	-6.16	1.44	1.52
1	A	265	GLN	CD-NE2	-6.13	1.20	1.33
1	A	124	ARG	CD-NE	-6.13	1.37	1.46
1	A	168	TYR	C-O	6.13	1.30	1.24
1	A	85	PHE	CA-C	6.12	1.60	1.52
1	A	81	GLY	C-N	6.09	1.42	1.33
1	A	225	ARG	CG-CD	6.09	1.70	1.52
1	A	195	VAL	C-N	-5.98	1.25	1.33
1	A	21	PHE	CA-CB	-5.98	1.45	1.53
1	A	191	TRP	CE2-CZ2	5.92	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	ARG	CZ-NH1	5.91	1.41	1.32
1	A	239	THR	C-O	5.86	1.31	1.24
1	A	141	VAL	N-CA	5.84	1.53	1.46
1	A	28	PHE	C-O	5.81	1.31	1.24
1	A	289	ARG	NE-CZ	5.80	1.39	1.33
1	A	256	PRO	CA-C	5.80	1.60	1.52
1	A	189	GLY	CA-C	-5.77	1.45	1.51
1	A	323	ARG	CZ-NH2	-5.71	1.26	1.33
1	A	6	TYR	CA-C	-5.70	1.45	1.52
1	A	5	CYS	CA-CB	-5.64	1.45	1.53
1	A	93	GLN	C-O	5.63	1.30	1.24
1	A	235	MET	C-N	-5.58	1.27	1.33
1	A	357	ASP	CB-CG	5.56	1.66	1.52
1	A	269	GLU	CA-CB	-5.51	1.44	1.53
1	A	62	LEU	N-CA	5.51	1.53	1.46
1	A	357	ASP	N-CA	5.46	1.52	1.46
1	A	91	LYS	N-CA	-5.45	1.39	1.46
1	A	206	GLU	CA-CB	5.44	1.60	1.52
1	A	290	PHE	CA-C	5.43	1.59	1.52
1	A	300	LYS	CA-CB	5.41	1.63	1.53
1	A	20	CYS	N-CA	5.41	1.52	1.46
1	A	33	VAL	C-O	5.41	1.30	1.24
1	A	314	LYS	CD-CE	-5.35	1.36	1.52
1	A	300	LYS	CB-CG	-5.34	1.36	1.52
1	A	359	LEU	CB-CG	-5.30	1.42	1.53
1	A	103	PRO	C-O	5.26	1.30	1.24
1	A	5	CYS	C-N	-5.23	1.26	1.33
1	A	63	LYS	CB-CG	-5.21	1.36	1.52
1	A	357	ASP	CG-OD2	5.19	1.35	1.25
1	A	244	TYR	CA-C	-5.17	1.46	1.52
1	A	245	THR	CA-C	5.17	1.59	1.52
1	A	305	VAL	CA-CB	5.16	1.61	1.54
1	A	51	ASN	N-CA	5.12	1.52	1.46
1	A	243	SER	C-N	-5.09	1.26	1.33
1	A	267	THR	C-N	-5.07	1.26	1.33
1	A	82	SER	N-CA	5.07	1.52	1.46
1	A	31	THR	C-N	-5.05	1.26	1.33
1	A	319	TYR	CA-C	-5.04	1.46	1.52
1	A	192	ARG	N-CA	-5.02	1.39	1.45
1	A	84	ARG	NE-CZ	-5.01	1.27	1.33
1	A	127	ARG	CZ-NH1	5.00	1.39	1.32
1	A	359	LEU	C-O	5.00	1.30	1.24

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	O-C-N	-12.73	108.62	122.12
1	A	192	ARG	CA-C-N	-11.96	103.04	123.25
1	A	192	ARG	C-N-CA	-11.96	103.04	123.25
1	A	225	ARG	NE-CZ-NH2	9.95	128.15	119.20
1	A	357	ASP	CA-CB-CG	9.64	122.24	112.60
1	A	61	THR	CA-C-N	9.51	134.26	120.38
1	A	61	THR	C-N-CA	9.51	134.26	120.38
1	A	357	ASP	N-CA-C	-8.76	101.69	111.07
1	A	300	LYS	CG-CD-CE	8.29	130.38	111.30
1	A	212	ARG	N-CA-C	8.22	122.87	113.01
1	A	323	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	A	84	ARG	CA-C-O	7.99	129.02	120.55
1	A	61	THR	OG1-CB-CG2	7.84	124.99	109.30
1	A	142	ARG	CD-NE-CZ	7.40	134.76	124.40
1	A	91	LYS	CD-CE-NZ	7.31	135.30	111.90
1	A	12	GLN	N-CA-C	7.00	119.76	111.71
1	A	26	ASP	O-C-N	7.00	127.69	121.18
1	A	170	ILE	O-C-N	7.00	128.66	121.87
1	A	97	THR	O-C-N	-6.96	114.91	122.07
1	A	170	ILE	CA-C-O	-6.93	113.74	120.95
1	A	62	LEU	N-CA-CB	6.88	121.02	110.14
1	A	62	LEU	N-CA-C	-6.86	102.97	111.75
1	A	327	GLY	CA-C-O	6.86	127.22	121.05
1	A	61	THR	N-CA-C	-6.76	104.89	113.01
1	A	36	SER	O-C-N	-6.65	114.59	123.23
1	A	84	ARG	CA-C-N	6.64	129.71	120.29
1	A	84	ARG	C-N-CA	6.64	129.71	120.29
1	A	356	LYS	CA-C-N	6.64	129.07	120.44
1	A	356	LYS	C-N-CA	6.64	129.07	120.44
1	A	84	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	A	300	LYS	N-CA-C	-6.45	97.73	108.75
1	A	87	LYS	CB-CG-CD	6.41	126.03	111.30
1	A	192	ARG	O-C-N	-6.35	114.83	122.65
1	A	225	ARG	CB-CG-CD	6.35	125.91	111.30
1	A	359	LEU	CA-C-O	-6.29	112.74	119.97
1	A	88	ILE	N-CA-C	6.21	116.99	110.72
1	A	3	LEU	O-C-N	6.11	132.27	122.99
1	A	60	ASN	CB-CA-C	6.10	122.38	110.67
1	A	141	VAL	O-C-N	-6.06	115.99	121.87
1	A	50	TRP	O-C-N	6.04	128.52	122.12
1	A	66	ASN	OD1-CG-ND2	5.98	128.58	122.60
1	A	51	ASN	O-C-N	-5.95	114.94	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	VAL	CA-C-O	-5.91	114.59	120.85
1	A	83	GLN	N-CA-CB	5.87	118.75	110.12
1	A	85	PHE	CA-C-O	5.86	126.63	120.42
1	A	20	CYS	CB-CA-C	5.86	119.47	110.62
1	A	265	GLN	CG-CD-NE2	-5.83	107.66	116.40
1	A	275	TYR	O-C-N	-5.69	116.09	122.12
1	A	123	TRP	CA-C-O	5.64	126.52	120.20
1	A	302	ASN	O-C-N	-5.62	115.35	122.26
1	A	39	ASN	OD1-CG-ND2	5.61	128.21	122.60
1	A	336	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	328	ALA	CA-C-O	-5.56	114.87	121.16
1	A	320	LEU	N-CA-C	-5.46	105.34	112.23
1	A	49	GLU	CG-CD-OE1	5.44	130.92	118.40
1	A	193	GLN	CB-CA-C	5.42	120.72	111.46
1	A	227	GLY	N-CA-C	5.41	122.78	115.00
1	A	240	PHE	O-C-N	5.34	128.94	122.85
1	A	28	PHE	CA-C-N	5.33	127.87	120.63
1	A	28	PHE	C-N-CA	5.33	127.87	120.63
1	A	302	ASN	CA-C-O	5.30	126.20	119.95
1	A	24	ALA	N-CA-C	-5.30	106.65	113.01
1	A	60	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	3	LEU	CA-C-O	-5.29	113.17	120.52
1	A	157	VAL	CA-C-N	5.28	125.21	119.78
1	A	157	VAL	C-N-CA	5.28	125.21	119.78
1	A	4	ILE	CA-CB-CG1	5.25	119.33	110.40
1	A	108	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	46	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	119	LEU	O-C-N	-5.18	116.09	122.82
1	A	204	GLY	CA-C-N	-5.17	112.98	121.92
1	A	204	GLY	C-N-CA	-5.17	112.98	121.92
1	A	263	PRO	O-C-N	5.16	129.16	122.91
1	A	118	TRP	CA-C-O	-5.11	114.54	120.62
1	A	243	SER	CA-C-O	-5.10	115.39	121.16
1	A	58	THR	N-CA-C	-5.07	105.75	111.28
1	A	38	ALA	CA-C-O	-5.03	115.33	121.36
1	A	93	GLN	O-C-N	-5.00	115.73	122.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	300	LYS	Mainchain
1	A	80	PHE	Sidechain

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	A	2883	0	2811	10	0
2	B	28	0	25	0	0
3	A	8	0	14	0	0
4	A	4	0	6	2	0
5	A	413	0	0	5	0
All	All	3336	0	2856	10	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 2.

All (10) 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:A:127:ARG:NH2	5:A:505:HOH:O	2.26	0.69
1:A:57:ASP:O	1:A:61:THR:HG23	1.95	0.66
1:A:78:TRP:HZ3	4:A:404:ACN:H22	1.60	0.65
1:A:269:GLU:OE2	5:A:501:HOH:O	2.14	0.64
1:A:78:TRP:CZ3	4:A:404:ACN:H22	2.36	0.60
1:A:70:LYS:HE2	5:A:587:HOH:O	2.04	0.56
1:A:357:ASP:HB2	5:A:649:HOH:O	2.05	0.56
1:A:286:THR:HG22	1:A:288:HIS:NE2	2.26	0.51
1:A:205:GLN:HG3	1:A:292:ASP:OD2	2.15	0.46
1:A:149:GLU:OE1	5:A:503:HOH:O	2.22	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	A	361/361 (100%)	348 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	304/302 (101%)	297 (98%)	7 (2%)	44	16

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	83	GLN
1	A	91	LYS
1	A	184	THR
1	A	203	ARG
1	A	225	ARG
1	A	362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	265	GLN
1	A	310	GLN
1	A	345	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	B	1	2,1	14,14,15	3.32	6 (42%)	17,19,21	2.75	9 (52%)
2	NAG	B	2	2	14,14,15	1.64	4 (28%)	17,19,21	2.49	8 (47%)

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	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	-6.79	1.43	1.52
2	B	1	NAG	O5-C1	-6.74	1.32	1.43
2	B	1	NAG	C4-C5	-4.65	1.43	1.53
2	B	1	NAG	O5-C5	4.02	1.51	1.43
2	B	1	NAG	O4-C4	3.80	1.52	1.43
2	B	2	NAG	C1-C2	3.59	1.57	1.52
2	B	2	NAG	C3-C2	-2.66	1.46	1.52
2	B	1	NAG	C3-C2	2.62	1.58	1.52
2	B	2	NAG	O3-C3	2.44	1.49	1.43
2	B	2	NAG	C2-N2	-2.20	1.42	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C4-C3-C2	-5.40	103.11	111.02
2	B	2	NAG	C1-O5-C5	5.03	118.93	112.19
2	B	2	NAG	C4-C3-C2	-5.01	103.68	111.02
2	B	1	NAG	C2-N2-C7	-4.20	117.27	122.90
2	B	1	NAG	O5-C5-C4	-3.89	101.37	110.83
2	B	1	NAG	C1-O5-C5	-3.61	107.34	112.19
2	B	2	NAG	O4-C4-C3	-3.44	102.26	110.38
2	B	1	NAG	C6-C5-C4	3.41	121.40	113.02
2	B	1	NAG	O5-C5-C6	-3.26	101.32	107.66
2	B	2	NAG	C1-C2-N2	3.03	115.21	110.43
2	B	2	NAG	O5-C5-C6	2.80	113.11	107.66
2	B	1	NAG	O4-C4-C3	-2.66	104.09	110.38
2	B	1	NAG	O7-C7-C8	-2.47	117.66	122.05
2	B	2	NAG	C6-C5-C4	-2.28	107.42	113.02
2	B	1	NAG	O4-C4-C5	-2.28	103.72	109.32
2	B	2	NAG	O3-C3-C2	2.25	114.08	109.40
2	B	2	NAG	O5-C5-C4	-2.02	105.92	110.83

There are no chirality outliers.

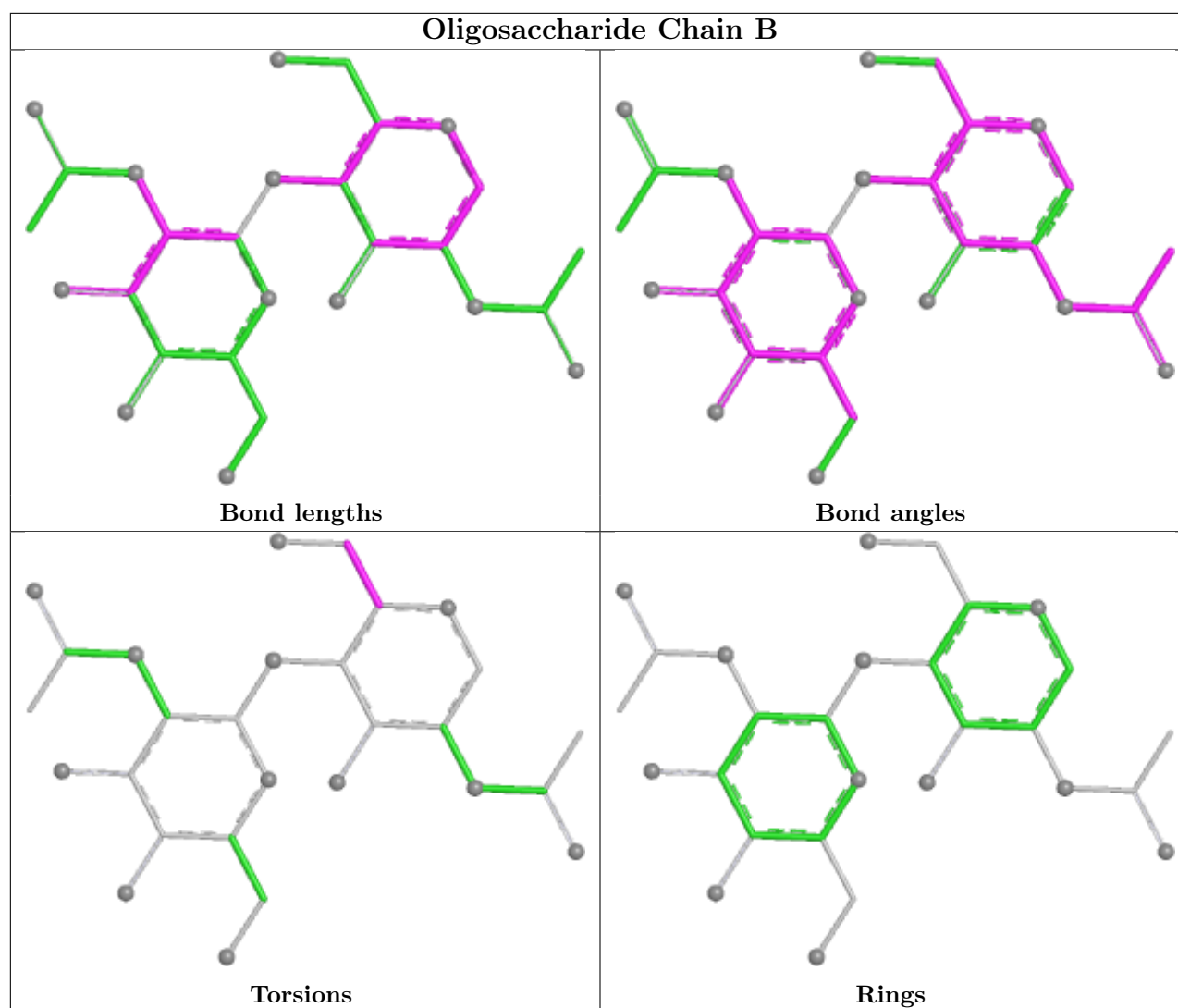
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	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](#)

2 ligands 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	$\# Z > 2$
3	MPD	A	401	-	7,7,7	2.31	2 (28%)	9,10,10	1.85	3 (33%)
4	ACN	A	404	-	3,3,3	0.93	0	3,3,3	1.44	0

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
3	MPD	A	401	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	MPD	C3-C2	-5.07	1.39	1.54
3	A	401	MPD	C1-C2	2.45	1.59	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	MPD	C1-C2-C3	3.24	124.16	110.20
3	A	401	MPD	O2-C2-C1	-3.04	98.53	107.99
3	A	401	MPD	O2-C2-CM	-2.25	100.97	107.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	MPD	C2-C3-C4-O4
3	A	401	MPD	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	ACN	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	A	361/361 (100%)	0.18	20 (5%)	30 33	14, 23, 42, 90	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	ALA	6.2
1	A	209	SER	5.2
1	A	81	GLY	4.5
1	A	362	VAL	4.3
1	A	210	SER	4.3
1	A	78	TRP	4.1
1	A	206	GLU	4.0
1	A	24	ALA	3.9
1	A	82	SER	3.5
1	A	191	TRP	3.5
1	A	80	PHE	3.4
1	A	20	CYS	3.4
1	A	207	ASP	3.2
1	A	120	TYR	2.6
1	A	21	PHE	2.5
1	A	205	GLN	2.5
1	A	361	GLY	2.4
1	A	360	ALA	2.1
1	A	48	TRP	2.1
1	A	247	ALA	2.0

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

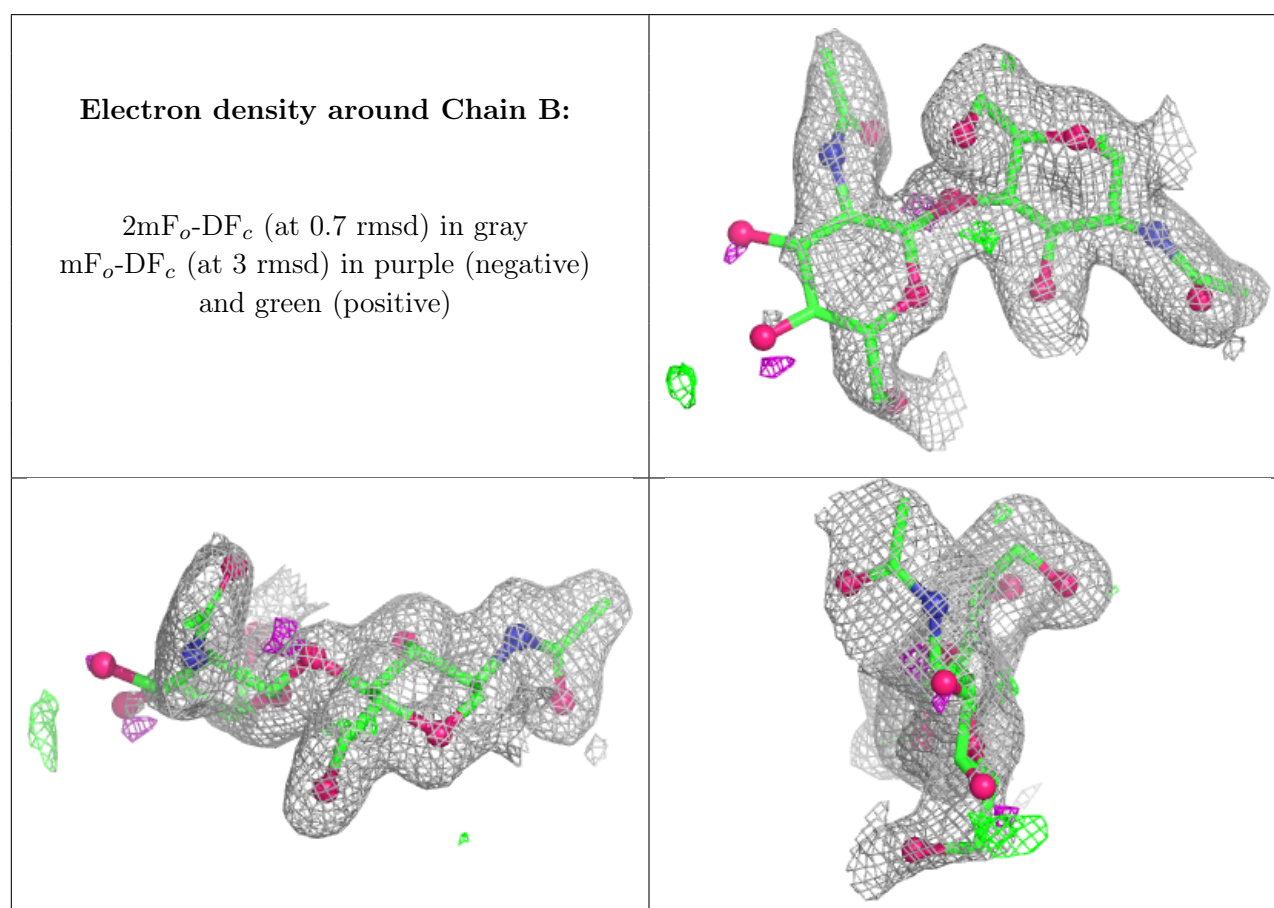
There are no non-standard protein/DNA/RNA residues in this entry.

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	B	2	14/15	0.77	0.14	45,54,59,61	0
2	NAG	B	1	14/15	0.93	0.08	25,31,37,39	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($\text{\AA}^2$)	Q<0.9
4	ACN	A	404	4/4	0.90	0.11	31,33,34,36	0
3	MPD	A	401	8/8	0.92	0.09	22,24,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.