



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:35 AM UTC

PDB ID : 8OPZ / pdb_00008opz
Title : Crystal structure of a tailspike depolymerase (APK16_gp47) from Acinetobacter phage APK16
Authors : Matyuta, I.O.; Boyko, K.M.; Nikolaeva, A.Y.; Shneider, M.M.; Timoshina, O.Y.; Miroshnikov, K.A.; Popov, V.O.
Deposited on : 2023-04-10
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

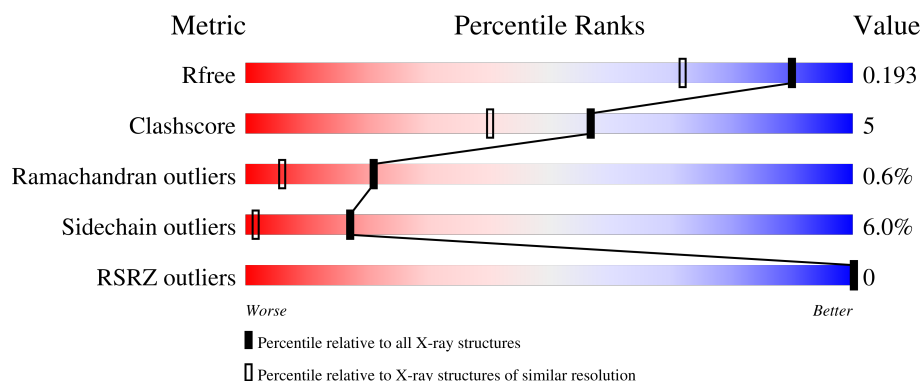
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
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	641	

2 Entry composition [i](#)

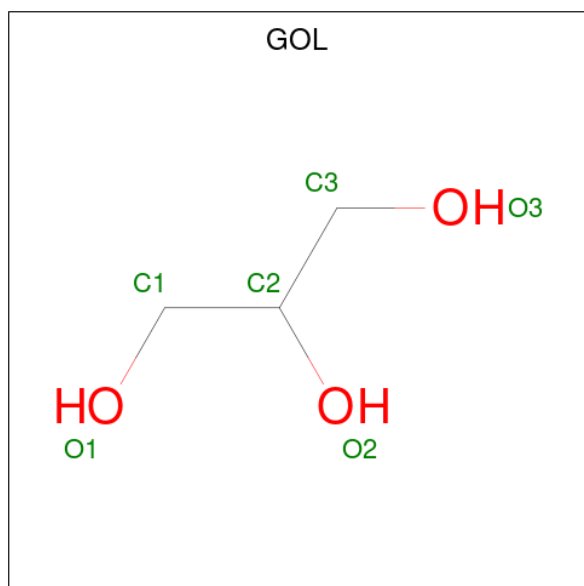
There are 3 unique types of molecules in this entry. The entry contains 4817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tailspike depolymerase (APK16_gp47) from Acinetobacter phage APK16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	4	0
			4733	2955	817	942	19			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

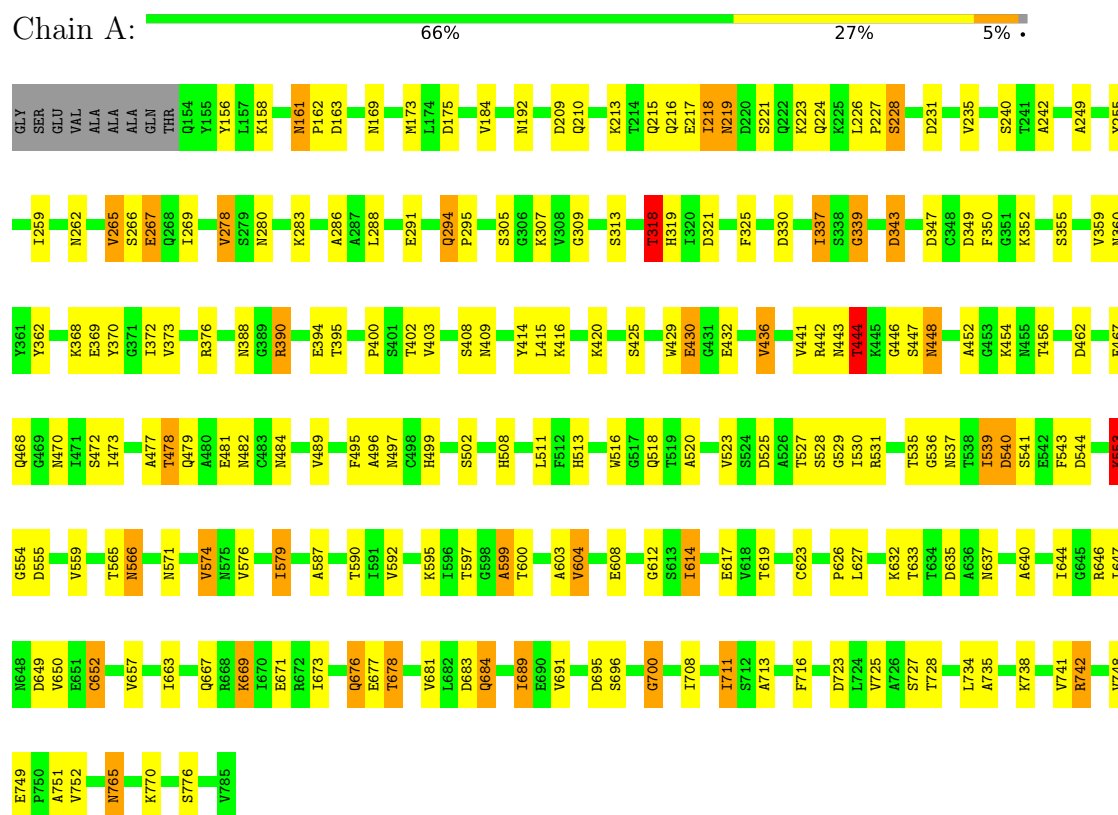
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		

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: Tailspike depolymerase (APK16_gp47) from Acinetobacter phage APK16



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	88.05Å 88.05Å 254.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.99 – 1.50 84.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.99-1.50) 99.8 (84.99-1.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.175 , 0.215 (Not available) , 0.193	Depositor DCC
R_{free} test set	5830 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 17.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.417 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: GOL

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	1.20	2/4836 (0.0%)	2.19	203/6576 (3.1%)

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	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	ASN	C-O	6.27	1.26	1.23
1	A	612	GLY	C-N	5.75	1.41	1.33

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	749	GLU	CB-CA-C	11.85	125.92	108.86
1	A	511	LEU	O-C-N	9.70	134.48	123.42
1	A	495	PHE	CA-CB-CG	9.62	123.42	113.80
1	A	544	ASP	CA-CB-CG	9.15	121.75	112.60
1	A	390	ARG	CD-NE-CZ	9.05	137.07	124.40
1	A	456	THR	CB-CA-C	8.77	124.40	110.19
1	A	337	ILE	N-CA-CB	8.63	122.62	112.35
1	A	633	THR	CB-CA-C	8.52	124.93	110.79
1	A	637	ASN	CB-CA-C	8.50	124.40	110.81
1	A	677	GLU	CB-CG-CD	8.13	126.43	112.60
1	A	343	ASP	CB-CA-C	8.07	123.68	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	GLY	CA-C-N	8.05	132.30	120.87
1	A	612	GLY	C-N-CA	8.05	132.30	120.87
1	A	671	GLU	CB-CA-C	8.00	123.16	110.19
1	A	667	GLN	CB-CA-C	7.91	123.18	109.65
1	A	349	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	649	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	349	ASP	CB-CA-C	7.55	122.86	110.78
1	A	741	VAL	N-CA-CB	7.44	119.48	111.00
1	A	565	THR	CB-CA-C	7.40	123.02	110.81
1	A	619	THR	CB-CA-C	7.07	121.42	109.75
1	A	330	ASP	CA-C-N	7.05	130.06	120.54
1	A	330	ASP	C-N-CA	7.05	130.06	120.54
1	A	227	PRO	CB-CA-C	7.03	120.50	111.64
1	A	529	GLY	O-C-N	7.00	131.80	122.70
1	A	695	ASP	CB-CA-C	6.99	121.61	109.65
1	A	390	ARG	CG-CD-NE	6.96	127.31	112.00
1	A	444	THR	CA-CB-OG1	6.91	119.96	109.60
1	A	725	VAL	N-CA-CB	6.87	118.21	110.72
1	A	402	THR	O-C-N	6.81	125.87	120.83
1	A	684	GLN	CB-CA-C	6.78	120.47	109.90
1	A	213	LYS	CA-C-N	6.77	130.97	120.75
1	A	213	LYS	C-N-CA	6.77	130.97	120.75
1	A	708	ILE	O-C-N	6.77	130.22	123.18
1	A	319	HIS	CB-CA-C	6.72	120.90	110.14
1	A	579	ILE	CB-CA-C	6.67	119.66	110.99
1	A	368	LYS	CB-CA-C	6.66	121.64	110.79
1	A	723	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	169	ASN	CB-CA-C	6.62	119.60	110.06
1	A	663	ILE	CA-C-O	-6.61	113.39	120.59
1	A	350	PHE	CA-CB-CG	6.60	120.40	113.80
1	A	339	GLY	O-C-N	6.60	128.51	122.18
1	A	161	ASN	CB-CA-C	6.53	117.66	110.15
1	A	242	ALA	CA-C-N	6.53	129.35	120.54
1	A	242	ALA	C-N-CA	6.53	129.35	120.54
1	A	163	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	776	SER	CA-C-N	6.50	131.84	122.21
1	A	776	SER	C-N-CA	6.50	131.84	122.21
1	A	477	ALA	CA-C-N	6.44	128.92	120.28
1	A	477	ALA	C-N-CA	6.44	128.92	120.28
1	A	592	VAL	O-C-N	6.35	130.53	123.10
1	A	283	LYS	CB-CA-C	6.33	120.11	109.48
1	A	373	VAL	CB-CA-C	6.31	119.74	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	GLU	CB-CG-CD	6.31	123.33	112.60
1	A	511	LEU	CA-C-N	-6.30	113.31	122.19
1	A	511	LEU	C-N-CA	-6.30	113.31	122.19
1	A	553	LYS	CB-CA-C	6.29	120.67	109.65
1	A	723	ASP	CB-CA-C	6.29	121.04	110.79
1	A	470	ASN	CB-CA-C	6.29	120.75	110.88
1	A	216	GLN	CA-C-N	6.27	128.69	120.28
1	A	216	GLN	C-N-CA	6.27	128.69	120.28
1	A	614	ILE	CA-C-O	6.27	126.91	120.39
1	A	677	GLU	CA-C-N	6.20	133.38	121.54
1	A	677	GLU	C-N-CA	6.20	133.38	121.54
1	A	448	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	540	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	555	ASP	CB-CA-C	-6.14	99.52	109.72
1	A	608	GLU	CB-CG-CD	6.13	123.03	112.60
1	A	473	ILE	CB-CA-C	6.12	119.17	110.84
1	A	219	ASN	CA-CB-CG	6.03	118.63	112.60
1	A	278	VAL	CA-CB-CG1	6.02	120.63	110.40
1	A	409	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	600	THR	CB-CA-C	5.98	120.38	110.81
1	A	388	ASN	O-C-N	5.97	130.20	123.27
1	A	689	ILE	CB-CA-C	5.97	119.46	110.63
1	A	657	VAL	O-C-N	5.96	129.52	123.20
1	A	467	GLU	CB-CG-CD	5.93	122.69	112.60
1	A	330	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	604	VAL	O-C-N	5.91	129.42	123.10
1	A	231	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	372	ILE	O-C-N	5.91	127.85	121.94
1	A	489	VAL	O-C-N	5.90	129.44	123.07
1	A	265	VAL	CA-CB-CG1	5.89	120.42	110.40
1	A	444	THR	N-CA-CB	-5.89	100.34	111.00
1	A	184	VAL	CA-C-N	5.88	130.67	120.68
1	A	184	VAL	C-N-CA	5.88	130.67	120.68
1	A	735	ALA	CA-C-N	5.85	130.74	122.09
1	A	735	ALA	C-N-CA	5.85	130.74	122.09
1	A	691	VAL	O-C-N	5.84	129.57	123.26
1	A	700	GLY	CA-C-N	5.83	128.90	120.38
1	A	700	GLY	C-N-CA	5.83	128.90	120.38
1	A	321	ASP	CB-CA-C	5.83	121.11	111.31
1	A	644	ILE	CA-CB-CG1	5.83	120.31	110.40
1	A	683	ASP	CA-C-N	5.83	129.03	120.82
1	A	683	ASP	C-N-CA	5.83	129.03	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	GLU	CB-CG-CD	5.82	122.49	112.60
1	A	676	GLN	CA-C-N	5.82	128.01	120.44
1	A	676	GLN	C-N-CA	5.82	128.01	120.44
1	A	566	ASN	CB-CA-C	5.82	116.06	111.00
1	A	635	ASP	CA-C-N	5.81	128.34	120.38
1	A	635	ASP	C-N-CA	5.81	128.34	120.38
1	A	632	LYS	CA-C-N	5.80	128.05	120.28
1	A	632	LYS	C-N-CA	5.80	128.05	120.28
1	A	652	CYS	CB-CA-C	5.80	119.57	109.65
1	A	742	ARG	CB-CG-CD	5.80	124.63	111.30
1	A	352	LYS	N-CA-CB	5.79	120.42	110.68
1	A	156	TYR	CB-CA-C	5.79	119.68	110.19
1	A	531	ARG	CG-CD-NE	5.74	124.62	112.00
1	A	650	VAL	N-CA-CB	5.73	119.08	112.15
1	A	224	GLN	CB-CA-C	5.72	122.38	110.32
1	A	592	VAL	CA-C-O	-5.71	114.42	120.53
1	A	599	ALA	CA-C-N	5.71	128.25	120.54
1	A	599	ALA	C-N-CA	5.71	128.25	120.54
1	A	436	VAL	CA-C-N	-5.71	114.82	122.42
1	A	436	VAL	C-N-CA	-5.71	114.82	122.42
1	A	265	VAL	CB-CA-C	5.70	118.86	110.77
1	A	752	VAL	CA-CB-CG2	5.70	120.09	110.40
1	A	595	LYS	N-CA-CB	5.69	119.49	110.84
1	A	728	THR	CA-C-N	5.68	128.98	120.69
1	A	728	THR	C-N-CA	5.68	128.98	120.69
1	A	559	VAL	CA-CB-CG2	5.67	120.03	110.40
1	A	228	SER	O-C-N	5.66	130.40	123.10
1	A	751	ALA	O-C-N	5.65	128.11	122.12
1	A	540	ASP	N-CA-CB	5.64	120.00	110.46
1	A	402	THR	CA-C-N	5.61	130.12	121.71
1	A	402	THR	C-N-CA	5.61	130.12	121.71
1	A	531	ARG	CA-C-N	-5.60	114.87	122.77
1	A	531	ARG	C-N-CA	-5.60	114.87	122.77
1	A	531	ARG	O-C-N	5.58	129.69	123.05
1	A	291	GLU	CB-CG-CD	5.57	122.07	112.60
1	A	647	ILE	O-C-N	5.57	129.03	123.18
1	A	321	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	696	SER	CA-C-N	5.56	127.08	120.14
1	A	696	SER	C-N-CA	5.56	127.08	120.14
1	A	587	ALA	CA-C-N	5.55	125.45	119.85
1	A	587	ALA	C-N-CA	5.55	125.45	119.85
1	A	262	ASN	CB-CA-C	5.54	119.71	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASN	CB-CA-C	5.54	118.84	111.14
1	A	349	ASP	O-C-N	5.52	129.62	123.05
1	A	597	THR	CB-CA-C	5.50	119.24	109.72
1	A	604	VAL	CA-CB-CG2	5.50	119.74	110.40
1	A	218	ILE	N-CA-CB	5.47	116.95	110.55
1	A	748	VAL	CA-CB-CG2	5.43	119.63	110.40
1	A	265	VAL	CA-C-N	5.42	131.20	121.66
1	A	265	VAL	C-N-CA	5.42	131.20	121.66
1	A	402	THR	CA-CB-CG2	5.41	119.70	110.50
1	A	286	ALA	CA-C-N	5.41	131.05	122.62
1	A	286	ALA	C-N-CA	5.41	131.05	122.62
1	A	217	GLU	N-CA-CB	5.40	118.06	110.12
1	A	711	ILE	CA-CB-CG2	5.39	119.66	110.50
1	A	537	ASN	CB-CA-C	5.37	118.63	109.72
1	A	325	PHE	CA-C-N	5.36	129.17	120.60
1	A	325	PHE	C-N-CA	5.36	129.17	120.60
1	A	468	GLN	O-C-N	5.36	125.94	122.03
1	A	637	ASN	CA-C-N	5.35	127.71	120.38
1	A	637	ASN	C-N-CA	5.35	127.71	120.38
1	A	749	GLU	N-CA-CB	-5.35	103.56	110.03
1	A	359	VAL	N-CA-CB	5.34	119.28	112.34
1	A	269	ILE	CA-C-N	5.33	129.49	122.30
1	A	269	ILE	C-N-CA	5.33	129.49	122.30
1	A	240	SER	CA-C-N	5.30	128.15	120.79
1	A	240	SER	C-N-CA	5.30	128.15	120.79
1	A	716	PHE	CB-CA-C	5.29	118.44	109.55
1	A	362	TYR	CB-CA-C	5.28	117.76	110.16
1	A	741	VAL	CA-CB-CG1	5.27	119.36	110.40
1	A	267	GLU	CB-CG-CD	5.27	121.55	112.60
1	A	543	PHE	N-CA-C	5.24	117.16	109.24
1	A	226	LEU	O-C-N	-5.22	116.31	121.17
1	A	535	THR	CA-CB-CG2	5.22	119.38	110.50
1	A	600	THR	CA-C-N	5.21	134.38	123.12
1	A	600	THR	C-N-CA	5.21	134.38	123.12
1	A	318	THR	CB-CA-C	5.18	119.61	109.35
1	A	221	SER	N-CA-CB	5.18	117.83	110.16
1	A	482	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	520	ALA	CA-C-N	5.17	128.55	120.75
1	A	520	ALA	C-N-CA	5.17	128.55	120.75
1	A	158	LYS	CB-CA-C	5.15	118.55	109.80
1	A	671	GLU	CB-CG-CD	5.14	121.35	112.60
1	A	249	ALA	CA-C-O	-5.14	115.08	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	THR	CA-CB-CG2	5.14	119.24	110.50
1	A	603	ALA	O-C-N	5.14	127.58	122.08
1	A	443	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	499	HIS	O-C-N	5.12	129.58	123.13
1	A	235	VAL	N-CA-C	5.08	115.23	108.11
1	A	400	PRO	CA-C-N	5.08	130.54	121.75
1	A	400	PRO	C-N-CA	5.08	130.54	121.75
1	A	640	ALA	O-C-N	5.07	129.24	122.95
1	A	444	THR	CA-CB-CG2	5.06	119.11	110.50
1	A	395	THR	CB-CA-C	5.06	119.03	109.37
1	A	436	VAL	CA-CB-CG2	5.05	118.99	110.40
1	A	590	THR	CA-CB-OG1	5.05	117.18	109.60
1	A	752	VAL	CA-CB-CG1	5.05	118.99	110.40
1	A	765	ASN	CA-C-N	5.05	130.56	120.77
1	A	765	ASN	C-N-CA	5.05	130.56	120.77
1	A	614	ILE	CA-CB-CG2	5.04	119.07	110.50
1	A	518	GLN	CA-C-N	5.04	128.00	120.90
1	A	518	GLN	C-N-CA	5.04	128.00	120.90
1	A	462	ASP	CB-CA-C	5.03	119.24	111.95
1	A	403	VAL	N-CA-C	-5.02	102.38	109.21
1	A	525	ASP	CA-C-N	5.02	127.01	120.28
1	A	525	ASP	C-N-CA	5.02	127.01	120.28
1	A	574	VAL	O-C-N	5.02	128.40	123.18
1	A	441	VAL	CG1-CB-CG2	-5.00	99.79	110.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	MET	Peptide
1	A	294	GLN	Peptide
1	A	539	ILE	Peptide
1	A	579	ILE	Peptide
1	A	669	LYS	Peptide
1	A	676	GLN	Peptide
1	A	700	GLY	Peptide
1	A	713	ALA	Peptide
1	A	738	LYS	Peptide

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	4733	0	4575	43	0
2	A	6	0	8	0	0
3	A	78	0	0	0	0
All	All	4817	0	4583	43	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 5.

All (43) 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:360:ASN:HD21	1:A:369:GLU:HA	1.54	0.73
1:A:484:ASN:HD22	1:A:508:HIS:H	1.39	0.70
1:A:318:THR:HG22	1:A:355:SER:HB3	1.79	0.64
1:A:209:ASP:HB2	1:A:218:ILE:HD11	1.79	0.64
1:A:318:THR:HG21	1:A:339:GLY:CA	2.34	0.57
1:A:444:THR:HG21	1:A:448:ASN:HA	1.87	0.56
1:A:536:GLY:HA2	1:A:571:ASN:O	2.07	0.55
1:A:228:SER:HA	1:A:255:TYR:O	2.07	0.54
1:A:496:ALA:HA	1:A:528:SER:O	2.07	0.53
1:A:318:THR:HG21	1:A:339:GLY:HA3	1.90	0.52
1:A:309:GLY:HA2	1:A:347:ASP:O	2.10	0.52
1:A:523:VAL:HG22	1:A:553:LYS:HG3	1.90	0.52
1:A:623:CYS:O	1:A:652:CYS:HA	2.10	0.52
1:A:604:VAL:O	1:A:627:LEU:HA	2.10	0.52
1:A:278:VAL:HG22	1:A:313:SER:HB3	1.92	0.51
1:A:541:SER:HB3	1:A:576:VAL:HG22	1.91	0.51
1:A:414:TYR:HE1	1:A:416:LYS:HE3	1.76	0.50
1:A:617:GLU:HA	1:A:646:ARG:O	2.12	0.50
1:A:215:GLN:HE21	1:A:219:ASN:HD21	1.59	0.50
1:A:420:LYS:HA	1:A:442:ARG:O	2.14	0.48
1:A:175:ASP:H	1:A:192:ASN:HD21	1.62	0.47
1:A:484:ASN:ND2	1:A:508:HIS:H	2.09	0.47
1:A:454:LYS:HA	1:A:481:GLU:O	2.14	0.47
1:A:530:ILE:HG21	1:A:539:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:SER:HA	1:A:343:ASP:O	2.16	0.46
1:A:430:GLU:HG2	1:A:452:ALA:HB3	1.97	0.46
1:A:574:VAL:HG13	1:A:576:VAL:HG23	1.99	0.45
1:A:209:ASP:HB2	1:A:218:ILE:CD1	2.45	0.45
1:A:527:THR:O	1:A:554:GLY:HA3	2.18	0.44
1:A:681:VAL:H	1:A:684:GLN:HE21	1.65	0.43
1:A:727:SER:HB2	1:A:734:LEU:HG	2.01	0.43
1:A:360:ASN:ND2	1:A:370:TYR:H	2.16	0.43
1:A:425:SER:HA	1:A:447:SER:O	2.19	0.42
1:A:599:ALA:O	1:A:623:CYS:HA	2.20	0.42
1:A:681:VAL:H	1:A:684:GLN:NE2	2.18	0.42
1:A:497:ASN:ND2	1:A:516:TRP:HB3	2.35	0.41
1:A:513:HIS:HE1	1:A:541:SER:OG	2.03	0.41
1:A:415:LEU:HB2	1:A:429:TRP:CZ2	2.55	0.41
1:A:343:ASP:HA	1:A:376:ARG:O	2.20	0.41
1:A:161:ASN:HA	1:A:162:PRO:HD3	1.95	0.40
1:A:415:LEU:HB2	1:A:429:TRP:CH2	2.57	0.40
1:A:444:THR:HG22	1:A:446:GLY:O	2.21	0.40
1:A:432:GLU:HA	1:A:454:LYS:O	2.21	0.40

There are no symmetry-related clashes.

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	A	634/641 (99%)	596 (94%)	34 (5%)	4 (1%)	21 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	PRO
1	A	678	THR

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Mol	Chain	Res	Type
1	A	288	LEU
1	A	626	PRO

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	501/511 (98%)	471 (94%)	30 (6%)	17 2

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	223	LYS
1	A	259	ILE
1	A	265	VAL
1	A	266	SER
1	A	267	GLU
1	A	294	GLN
1	A	307	LYS
1	A	318	THR
1	A	337	ILE
1	A	390	ARG
1	A	408	SER
1	A	436	VAL
1	A	444	THR
1	A	472	SER
1	A	478	THR
1	A	479	GLN
1	A	502	SER
1	A	540	ASP
1	A	553	LYS
1	A	566	ASN
1	A	614	ILE
1	A	669	LYS
1	A	673	ILE

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Mol	Chain	Res	Type
1	A	678	THR
1	A	689	ILE
1	A	711	ILE
1	A	742	ARG
1	A	765	ASN
1	A	770	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	215	GLN
1	A	360	ASN
1	A	377	ASN
1	A	409	ASN
1	A	440	HIS
1	A	448	ASN
1	A	470	ASN
1	A	482	ASN
1	A	484	ASN
1	A	497	ASN
1	A	501	HIS
1	A	508	HIS
1	A	513	HIS
1	A	518	GLN
1	A	533	GLN
1	A	593	ASN
1	A	628	GLN
1	A	648	ASN
1	A	684	GLN
1	A	736	ASN
1	A	745	HIS

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand 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	$\# Z > 2$
2	GOL	A	801	-	5,5,5	0.44	0	5,5,5	0.84	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
2	GOL	A	801	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2

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 [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	632/641 (98%)	-0.46	0 100 100	14, 28, 42, 54	4 (0%)

There are no RSRZ outliers to report.

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](#)

There are no oligosaccharides in this entry.

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
2	GOL	A	801	6/6	0.98	0.04	25,27,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.