



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:27 PM UTC

PDB ID : 24QI / pdb_000024qi
Title : Crystal structure of a tailspike depolymerase (Belisarius_gp86) from Acinetobacter phage Belisarius
Authors : Matyuta, I.O.; Shneider, M.M.; Timoshina, O.Y.; Popov, V.O.; Boyko, K.M.
Deposited on : 2026-03-16
Resolution : 2.20 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

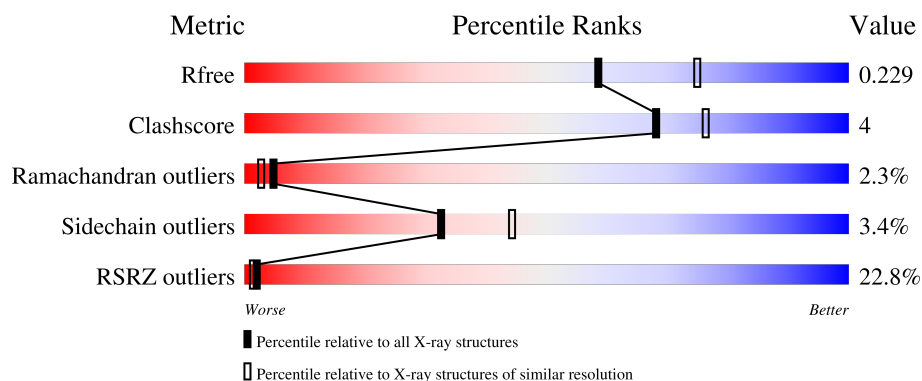
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	599	<div> <div>22%</div> <div>81%</div> <div>14%</div> <div>...</div> </div>

2 Entry composition [i](#)

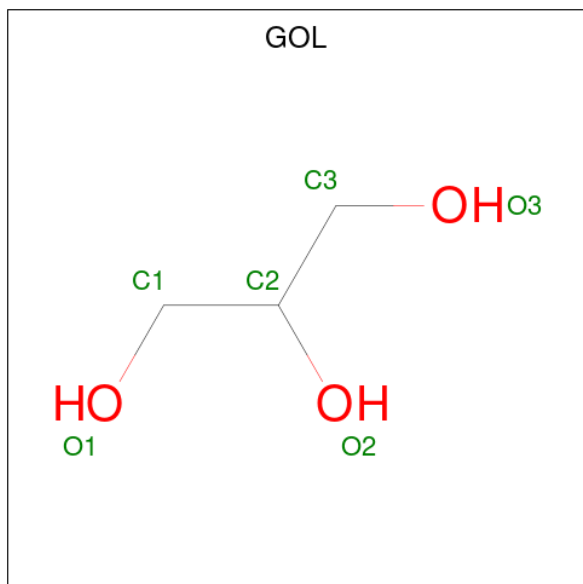
There are 4 unique types of molecules in this entry. The entry contains 4614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

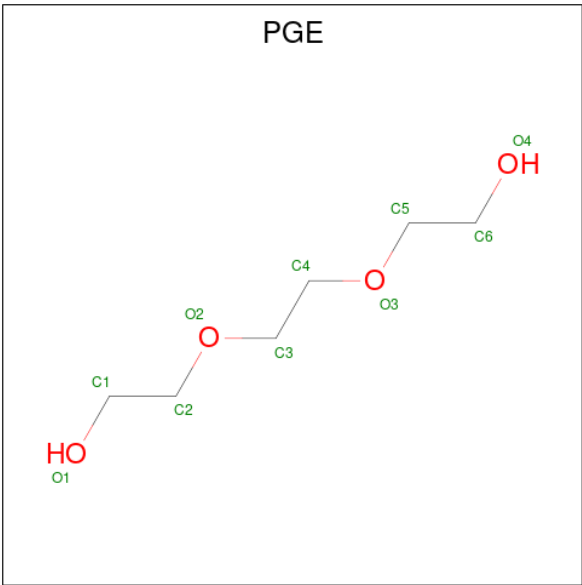
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	575	4409	2789	740	867	13	0	4	0

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



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

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		

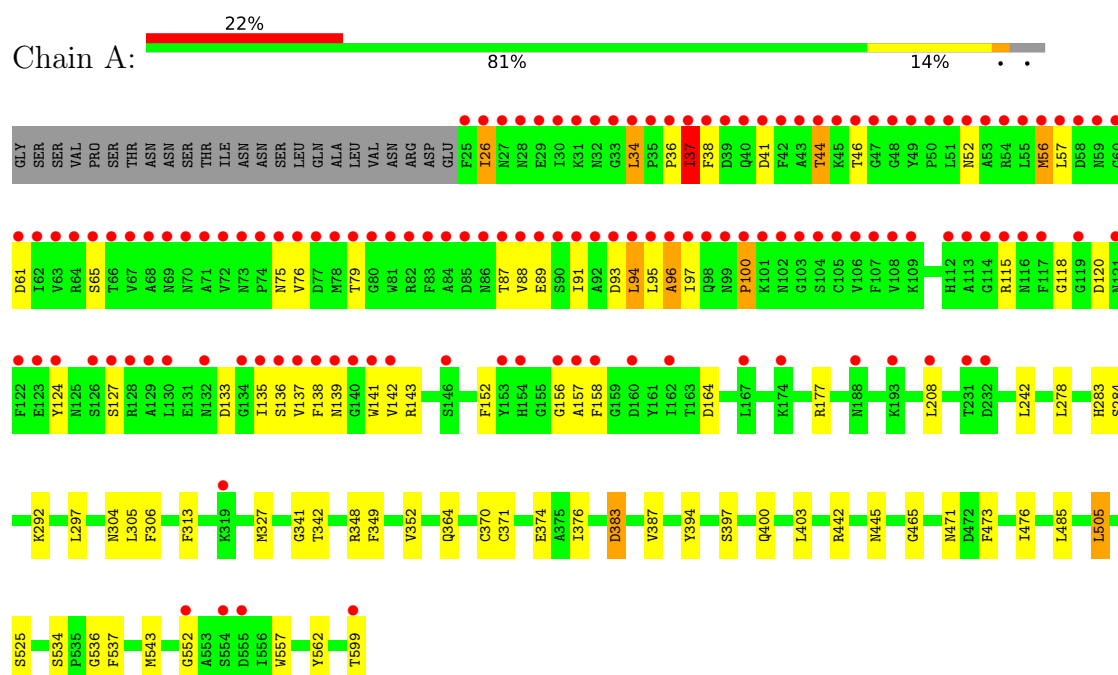
- Molecule 4 is water.

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

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: Tailspike depolymerase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.97Å 100.97Å 784.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.67 – 2.20 49.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.67-2.20) 99.6 (49.67-2.20)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.226 0.216 , 0.229	Depositor DCC
R_{free} test set	3996 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: PGE, 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	1.29	6/4520 (0.1%)	1.47	24/6146 (0.4%)

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	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	GLY	C-O	7.92	1.30	1.23
1	A	397	SER	C-O	6.78	1.32	1.23
1	A	278	LEU	C-O	5.81	1.31	1.24
1	A	525	SER	C-O	5.42	1.31	1.24
1	A	376	ILE	C-O	5.40	1.30	1.24
1	A	371	CYS	C-O	5.38	1.30	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	THR	CA-C-O	-6.38	109.95	120.80
1	A	177	ARG	CB-CA-C	-6.14	100.41	110.85
1	A	37	ILE	CB-CA-C	6.12	121.32	111.29
1	A	473	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	94	LEU	N-CA-C	-5.90	102.88	110.19
1	A	157	ALA	CA-C-N	5.88	132.77	121.54
1	A	157	ALA	C-N-CA	5.88	132.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	N-CA-CB	5.79	118.74	110.16
1	A	292	LYS	CB-CA-C	5.62	120.00	109.71
1	A	61	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	41	ASP	CA-C-N	5.46	128.35	120.38
1	A	41	ASP	C-N-CA	5.46	128.35	120.38
1	A	56	MET	CA-C-N	5.37	131.79	121.54
1	A	56	MET	C-N-CA	5.37	131.79	121.54
1	A	348	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	152	PHE	CA-C-N	5.32	127.41	120.28
1	A	152	PHE	C-N-CA	5.32	127.41	120.28
1	A	44	THR	CA-C-N	5.21	127.53	120.65
1	A	44	THR	C-N-CA	5.21	127.53	120.65
1	A	177	ARG	CG-CD-NE	-5.16	100.64	112.00
1	A	100	PRO	N-CA-CB	-5.13	97.87	103.25
1	A	476	ILE	CB-CA-C	5.11	117.79	110.33
1	A	536	GLY	CA-C-O	-5.08	118.66	122.37
1	A	94	LEU	CA-C-O	-5.05	116.70	122.01

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	GLY	Peptide
1	A	26	ILE	Peptide
1	A	552	GLY	Peptide
1	A	87	THR	Peptide
1	A	96	ALA	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	4409	0	4167	30	0
2	A	12	0	16	0	0
3	A	20	0	28	3	0
4	A	173	0	0	0	0
All	All	4614	0	4211	31	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 4.

All (31) 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:485:LEU:HD23	1:A:505:LEU:HD13	1.61	0.81
1:A:118:GLY:O	1:A:143:ARG:NH2	2.20	0.74
1:A:342:THR:HG23	3:A:604:PGE:H12	1.80	0.62
1:A:387:VAL:HG21	1:A:403:LEU:HD22	1.82	0.61
1:A:95:LEU:HD21	1:A:138:PHE:HB3	1.84	0.59
1:A:284:SER:HA	1:A:306:PHE:O	2.11	0.51
1:A:95:LEU:HD12	1:A:139:ASN:HD22	1.75	0.50
1:A:124:TYR:HB2	1:A:141:TRP:CZ2	2.49	0.48
1:A:543:MET:HA	1:A:557[B]:TRP:CE3	2.50	0.47
1:A:537:PHE:HA	1:A:562:TYR:O	2.15	0.47
1:A:124:TYR:HB2	1:A:141:TRP:CE2	2.50	0.47
1:A:94:LEU:C	1:A:96:ALA:H	2.23	0.46
1:A:133:ASP:OD2	1:A:136:SER:OG	2.30	0.46
1:A:137:VAL:HA	1:A:141:TRP:O	2.16	0.46
1:A:297:LEU:HB3	1:A:327:MET:HE2	1.98	0.46
1:A:313:PHE:O	1:A:349:PHE:HA	2.15	0.45
1:A:283:HIS:O	1:A:305:LEU:HA	2.17	0.45
1:A:445:ASN:HD22	1:A:471:ASN:HB2	1.80	0.44
1:A:305:LEU:O	1:A:341:GLY:HA3	2.18	0.44
1:A:89:GLU:HB2	1:A:93:ASP:OD2	2.18	0.43
1:A:364:GLN:HA	1:A:394:TYR:O	2.19	0.43
1:A:383:ASP:OD1	1:A:442[A]:ARG:NH2	2.52	0.43
1:A:124:TYR:HD2	1:A:141:TRP:CD1	2.38	0.42
1:A:370:CYS:HA	1:A:400:GLN:O	2.20	0.42
3:A:603:PGE:H2	3:A:603:PGE:H6	2.00	0.42
1:A:352:VAL:HA	1:A:374:GLU:O	2.20	0.41
1:A:137:VAL:HG23	1:A:142:VAL:HG22	2.02	0.41
1:A:403:LEU:C	1:A:403:LEU:HD12	2.45	0.41
1:A:304:ASN:OD1	3:A:604:PGE:H2	2.21	0.41
1:A:37:ILE:HG13	1:A:38:PHE:N	2.36	0.41
1:A:306:PHE:HA	1:A:342:THR:O	2.21	0.41

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	577/599 (96%)	520 (90%)	44 (8%)	13 (2%)	5 3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	36	PRO
1	A	52	ASN
1	A	56	MET
1	A	120	ASP
1	A	127	SER
1	A	164	ASP
1	A	57	LEU
1	A	75	ASN
1	A	158	PHE
1	A	100	PRO
1	A	34	LEU
1	A	135	ILE

5.3.2 Protein sidechains [i](#)

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	469/508 (92%)	453 (97%)	16 (3%)	32 44

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	37	ILE
1	A	44	THR
1	A	46	THR
1	A	65	SER
1	A	76	VAL
1	A	79	THR
1	A	88	VAL
1	A	91	ILE
1	A	97	ILE
1	A	115	ARG
1	A	208	LEU
1	A	242	LEU
1	A	383	ASP
1	A	505	LEU
1	A	534	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	139	ASN
1	A	217	ASN
1	A	255	ASN
1	A	324	ASN
1	A	356	GLN
1	A	430	GLN
1	A	445	ASN
1	A	471	ASN
1	A	548	ASN

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

4 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	PGE	A	603	-	9,9,9	0.59	0	8,8,8	0.41	0
2	GOL	A	601	-	5,5,5	0.25	0	5,5,5	0.42	0
3	PGE	A	604	-	9,9,9	0.98	0	8,8,8	0.75	0
2	GOL	A	602	-	5,5,5	0.89	0	5,5,5	1.21	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	PGE	A	603	-	-	2/7/7/7	-
2	GOL	A	601	-	-	2/4/4/4	-
3	PGE	A	604	-	-	2/7/7/7	-
2	GOL	A	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
3	A	604	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3
2	A	601	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
3	A	603	PGE	O3-C5-C6-O4
3	A	604	PGE	C6-C5-O3-C4
3	A	603	PGE	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	PGE	1	0
3	A	604	PGE	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 ⓘ

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	A	575/599 (95%)	1.12	131 (22%) 2 1	13, 42, 123, 177	4 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	ASP	11.3
1	A	68	ALA	10.3
1	A	71	ALA	9.2
1	A	58	ASP	9.1
1	A	26	ILE	9.0
1	A	41	ASP	8.9
1	A	30	ILE	8.9
1	A	38	PHE	8.9
1	A	29	GLU	8.2
1	A	56	MET	8.0
1	A	67	VAL	7.9
1	A	25	PHE	7.7
1	A	117	PHE	7.6
1	A	48	GLY	7.5
1	A	27	ASN	7.5
1	A	28	ASN	7.1
1	A	40	GLN	7.0
1	A	72	VAL	7.0
1	A	55	LEU	6.9
1	A	42	PHE	6.9
1	A	70	ASN	6.8
1	A	50	PRO	6.8
1	A	54	ARG	6.8
1	A	35	PRO	6.7
1	A	31	LYS	6.6
1	A	81	TRP	6.6
1	A	97	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	99	ASN	6.5
1	A	95	LEU	6.5
1	A	69	ASN	6.5
1	A	49	TYR	6.2
1	A	34	LEU	6.1
1	A	76	VAL	6.1
1	A	98	GLN	5.9
1	A	44	THR	5.9
1	A	37	ILE	5.6
1	A	75	ASN	5.6
1	A	93	ASP	5.6
1	A	62	ILE	5.5
1	A	33	GLY	5.4
1	A	87	THR	5.4
1	A	100	PRO	5.4
1	A	43	ALA	5.3
1	A	130	LEU	5.2
1	A	45	LYS	5.0
1	A	61	ASP	4.9
1	A	86	ASN	4.9
1	A	32	ASN	4.7
1	A	46	THR	4.7
1	A	83	PHE	4.6
1	A	51	LEU	4.6
1	A	84	ALA	4.5
1	A	127	SER	4.5
1	A	36	PRO	4.4
1	A	157	ALA	4.4
1	A	106	VAL	4.4
1	A	101	LYS	4.3
1	A	59	ASN	4.3
1	A	96	ALA	4.3
1	A	158	PHE	4.2
1	A	47	GLY	4.1
1	A	53	ALA	4.1
1	A	552	GLY	4.1
1	A	82	ARG	4.0
1	A	141	TRP	4.0
1	A	90	SER	3.9
1	A	60	GLY	3.8
1	A	126	SER	3.8
1	A	107	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	138	PHE	3.6
1	A	66	THR	3.6
1	A	52	ASN	3.6
1	A	114	GLY	3.5
1	A	115	ARG	3.4
1	A	124	TYR	3.4
1	A	63	VAL	3.4
1	A	105	CYS	3.4
1	A	142	VAL	3.3
1	A	57	LEU	3.3
1	A	94	LEU	3.3
1	A	79	THR	3.3
1	A	139	ASN	3.2
1	A	113	ALA	3.2
1	A	137	VAL	3.2
1	A	121	ASN	3.1
1	A	122	PHE	3.0
1	A	92	ALA	3.0
1	A	135	ILE	3.0
1	A	116	ASN	3.0
1	A	162	ILE	2.9
1	A	65	SER	2.9
1	A	78	MET	2.9
1	A	103	GLY	2.9
1	A	74	PRO	2.8
1	A	140	GLY	2.8
1	A	88	VAL	2.8
1	A	156	GLY	2.7
1	A	73	ASN	2.7
1	A	89	GLU	2.7
1	A	80	GLY	2.7
1	A	85	ASP	2.6
1	A	91	ILE	2.6
1	A	129	ALA	2.6
1	A	128	ARG	2.6
1	A	232	ASP	2.6
1	A	123	GLU	2.6
1	A	599	THR	2.6
1	A	174	LYS	2.5
1	A	64	ARG	2.4
1	A	108	VAL	2.4
1	A	208	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	109	LYS	2.4
1	A	112	HIS	2.4
1	A	102	ASN	2.3
1	A	153	TYR	2.3
1	A	134	GLY	2.3
1	A	188	ASN	2.3
1	A	193	LYS	2.3
1	A	146	SER	2.3
1	A	136	SER	2.2
1	A	160	ASP	2.2
1	A	119	GLY	2.2
1	A	154	HIS	2.2
1	A	77	ASP	2.1
1	A	132	ASN	2.1
1	A	104	SER	2.1
1	A	231	THR	2.0
1	A	167	LEU	2.0
1	A	319	LYS	2.0
1	A	554	SER	2.0
1	A	555	ASP	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](#)

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	601	6/6	0.74	0.31	59,70,90,93	0
3	PGE	A	603	10/10	0.78	0.36	47,77,111,115	0
2	GOL	A	602	6/6	0.83	0.21	37,40,44,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PGE	A	604	10/10	0.86	0.25	39,68,86,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.