



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:17 PM UTC

PDB ID : 8OQ0 / pdb_00008oq0
Title : Crystal structure of tailspike depolymerase (APK09_gp48) from Acinetobacter phage APK09
Authors : Matyuta, I.O.; Boyko, K.M.; Nikolaeva, A.Y.; Shneider, M.M.; Timoshina, O.Y.; Popova, A.V.; Miroshnikov, K.A.; Popov, V.O.
Deposited on : 2023-04-10
Resolution : 2.59 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

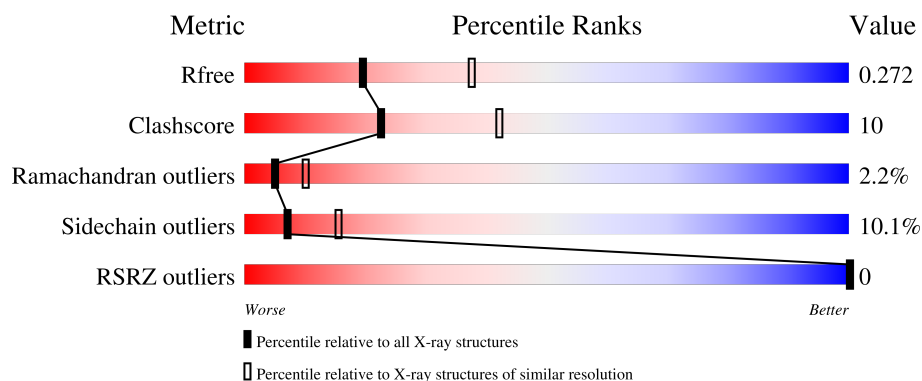
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	616	 63% 28% 6% ..

2 Entry composition [i](#)

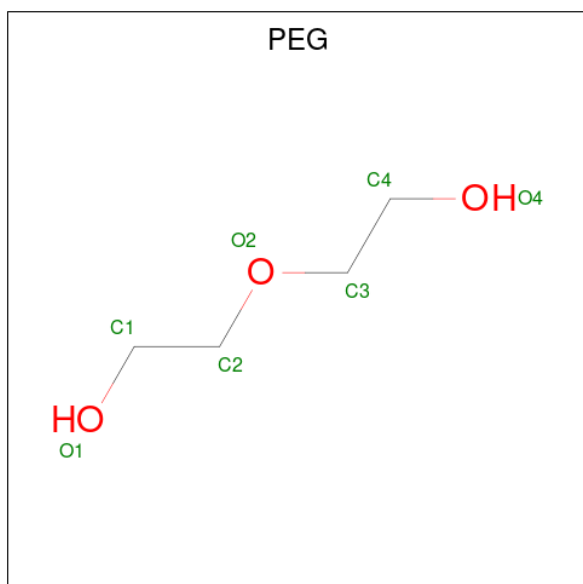
There are 3 unique types of molecules in this entry. The entry contains 4611 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	0	0
			4588	2892	771	905	20			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

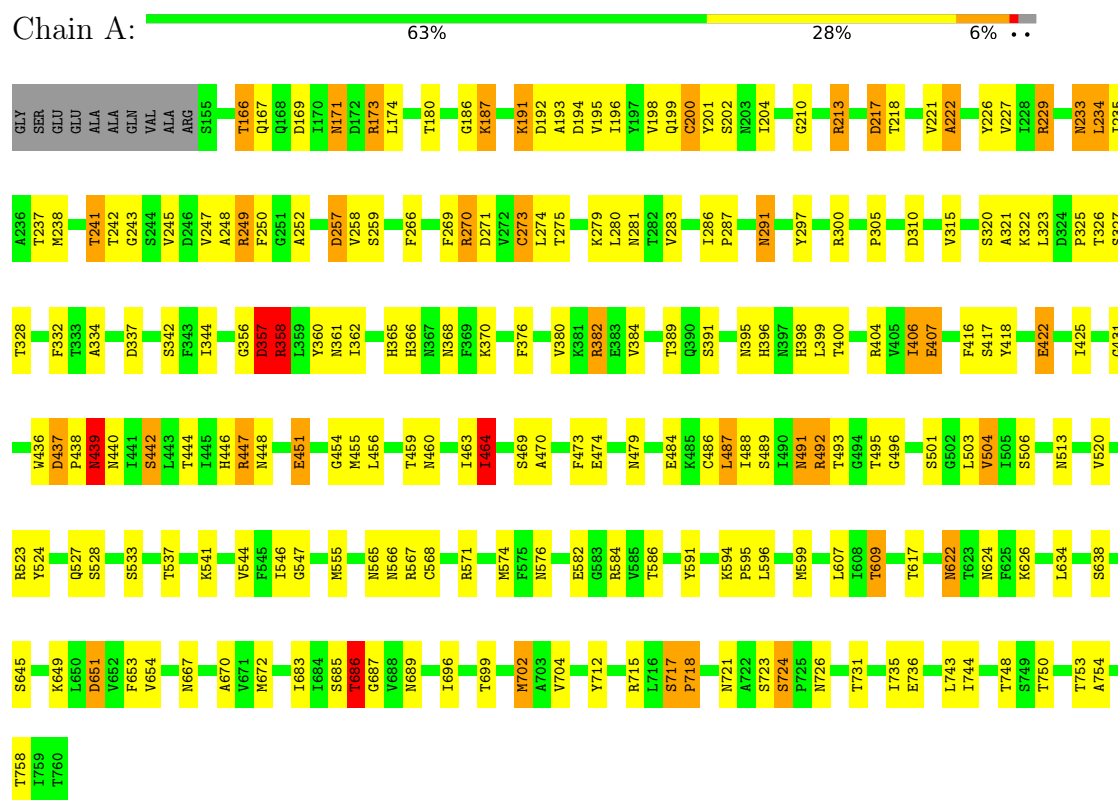
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

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 protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	88.69Å 88.69Å 421.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.15 – 2.59 72.15 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (72.15-2.59) 99.3 (72.15-2.59)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.272 0.189 , 0.272	Depositor DCC
R_{free} test set	1057 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.6	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	0.95	EDS
Total number of atoms	4611	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: PEG

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	0.79	0/4681	1.66	69/6381 (1.1%)

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	5

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	THR	CA-CB-OG1	-10.60	93.70	109.60
1	A	439	ASN	CB-CA-C	10.09	125.96	109.02
1	A	438	PRO	CB-CA-C	9.04	119.63	111.40
1	A	584	ARG	CG-CD-NE	8.39	130.46	112.00
1	A	241	THR	CB-CA-C	8.19	123.77	110.83
1	A	194	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	444	THR	CA-CB-OG1	-7.95	97.67	109.60
1	A	439	ASN	CA-CB-CG	7.78	120.38	112.60
1	A	270	ARG	CB-CA-C	7.59	121.33	109.03
1	A	492	ARG	CG-CD-NE	7.40	128.29	112.00
1	A	718	PRO	N-CA-C	7.11	127.12	112.47
1	A	493	THR	CB-CA-C	-7.09	98.58	109.99
1	A	495	THR	CB-CA-C	6.79	119.94	110.16
1	A	448	ASN	CA-CB-CG	-6.75	105.85	112.60
1	A	358	ARG	CB-CG-CD	6.56	126.39	111.30
1	A	696	ILE	CA-C-N	6.42	129.61	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	ILE	C-N-CA	6.42	129.61	122.55
1	A	491	ASN	CB-CA-C	6.37	122.22	110.24
1	A	328	THR	CA-CB-OG1	-6.36	100.07	109.60
1	A	582	GLU	CB-CA-C	-6.30	100.73	110.81
1	A	382	ARG	CG-CD-NE	-6.16	98.44	112.00
1	A	222	ALA	CA-C-N	6.15	129.14	120.28
1	A	222	ALA	C-N-CA	6.15	129.14	120.28
1	A	533	SER	CA-C-N	-6.15	112.50	122.82
1	A	533	SER	C-N-CA	-6.15	112.50	122.82
1	A	750	THR	CB-CA-C	6.10	122.56	110.42
1	A	440	ASN	CB-CA-C	-5.99	100.55	110.14
1	A	523	ARG	CG-CD-NE	-5.99	98.82	112.00
1	A	748	THR	CA-C-N	5.83	131.92	121.66
1	A	748	THR	C-N-CA	5.83	131.92	121.66
1	A	689	ASN	CB-CA-C	5.82	119.27	111.82
1	A	171	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	487	LEU	N-CA-CB	-5.79	102.02	110.47
1	A	754	ALA	CA-C-N	5.79	128.61	120.28
1	A	754	ALA	C-N-CA	5.79	128.61	120.28
1	A	437	ASP	CB-CA-C	5.78	121.56	110.17
1	A	332	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	217	ASP	N-CA-C	5.73	117.71	107.80
1	A	651	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	229	ARG	CB-CA-C	5.70	119.64	110.29
1	A	622	ASN	CA-CB-CG	-5.70	106.90	112.60
1	A	357	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	736	GLU	CB-CG-CD	5.54	122.01	112.60
1	A	537	THR	CA-CB-OG1	5.51	117.87	109.60
1	A	464	ILE	CB-CA-C	5.50	117.85	110.42
1	A	504	VAL	CB-CA-C	-5.49	102.65	110.83
1	A	416	PHE	CB-CA-C	5.44	118.83	111.70
1	A	496	GLY	CA-C-N	5.43	128.48	120.82
1	A	496	GLY	C-N-CA	5.43	128.48	120.82
1	A	696	ILE	CB-CA-C	5.43	118.64	110.98
1	A	192	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	218	THR	CB-CA-C	5.39	120.43	110.56
1	A	724	SER	CB-CA-C	5.38	115.93	109.31
1	A	653	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	271	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	270	ARG	CB-CG-CD	5.21	123.28	111.30
1	A	464	ILE	N-CA-CB	-5.20	104.75	111.82
1	A	609	THR	CB-CA-C	5.18	118.68	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	ASN	CA-C-N	5.15	126.58	120.14
1	A	513	ASN	C-N-CA	5.15	126.58	120.14
1	A	247	VAL	N-CA-C	-5.14	105.35	112.50
1	A	686	THR	CB-CA-C	5.08	120.00	110.70
1	A	193	ALA	CB-CA-C	5.08	114.86	109.83
1	A	233	ASN	CB-CA-C	5.07	118.95	110.44
1	A	210	GLY	CA-C-N	5.06	129.58	122.09
1	A	210	GLY	C-N-CA	5.06	129.58	122.09
1	A	473	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	382	ARG	CB-CG-CD	5.03	122.87	111.30
1	A	479	ASN	CB-CA-C	5.03	120.42	110.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	ASP	Peptide
1	A	437	ASP	Peptide
1	A	717	SER	Mainchain,Peptide
1	A	726	ASN	Peptide

5.2 Too-close contacts [i](#)

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	4588	0	4472	95	0
2	A	14	0	20	1	0
3	A	9	0	0	0	0
All	All	4611	0	4492	95	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 10.

All (95) 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:213:ARG:HH11	1:A:213:ARG:HG2	1.14	1.04
1:A:227:VAL:HG22	1:A:237:THR:HG22	1.45	0.97
1:A:431:GLY:HA3	1:A:439:ASN:OD1	1.77	0.85
1:A:506:SER:HB3	1:A:546:ILE:HG23	1.59	0.84
1:A:173:ARG:HH11	1:A:173:ARG:HG3	1.43	0.82
1:A:213:ARG:HG2	1:A:213:ARG:NH1	1.93	0.78
1:A:173:ARG:HH11	1:A:173:ARG:CG	2.03	0.71
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.00	0.71
1:A:173:ARG:HG3	1:A:173:ARG:NH1	2.10	0.65
1:A:281:ASN:HA	1:A:310:ASP:O	1.97	0.65
1:A:366:HIS:HA	1:A:396:HIS:O	1.97	0.64
1:A:486:CYS:SG	1:A:489:SER:HB2	2.40	0.62
1:A:672:MET:HB2	1:A:702:MET:HG2	1.83	0.61
1:A:376:PHE:HB2	1:A:406:ILE:HG12	1.81	0.61
1:A:356:GLY:HA3	1:A:389:THR:HG22	1.85	0.58
1:A:622:ASN:HB2	1:A:753:THR:HG23	1.84	0.57
1:A:395:ASN:HA	1:A:417:SER:O	2.05	0.57
1:A:463:ILE:O	1:A:464:ILE:HD13	2.04	0.56
1:A:702:MET:HE1	1:A:704:VAL:HG23	1.87	0.56
1:A:357:ASP:HB2	1:A:358:ARG:HD2	1.87	0.55
1:A:571:ARG:HA	1:A:574:MET:HE3	1.88	0.55
1:A:217:ASP:HB3	1:A:235:ILE:HG12	1.89	0.54
1:A:555:MET:HE3	1:A:568:CYS:HB3	1.90	0.54
1:A:486:CYS:HA	1:A:520:VAL:O	2.08	0.54
1:A:667:ASN:HA	1:A:712:TYR:OH	2.09	0.53
1:A:229:ARG:HA	1:A:235:ILE:HG22	1.90	0.53
1:A:257:ASP:HA	1:A:279:LYS:O	2.08	0.53
1:A:221:VAL:HG12	1:A:222:ALA:H	1.73	0.53
1:A:594:LYS:NZ	1:A:607:LEU:O	2.41	0.53
1:A:436:TRP:HB3	1:A:439:ASN:HB2	1.91	0.52
1:A:280:LEU:HD13	1:A:315:VAL:HG11	1.92	0.52
1:A:245:VAL:HG11	1:A:269:PHE:CD2	2.45	0.52
1:A:213:ARG:NH1	1:A:213:ARG:CG	2.65	0.51
1:A:201:TYR:CD2	1:A:202:SER:HB2	2.46	0.51
1:A:555:MET:HE1	1:A:566:ASN:HB3	1.92	0.50
1:A:459:THR:HG21	1:A:463:ILE:HD11	1.93	0.49
1:A:460:ASN:O	1:A:492:ARG:HA	2.13	0.48
1:A:238:MET:HG2	1:A:249:ARG:NH1	2.28	0.48
1:A:547:GLY:HA2	1:A:565:ASN:O	2.12	0.48
1:A:201:TYR:HD2	1:A:202:SER:HB2	1.78	0.48
1:A:166:THR:O	1:A:169:ASP:N	2.47	0.48
1:A:596:LEU:HA	1:A:599:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:HA	1:A:269:PHE:O	2.14	0.47
1:A:274:LEU:O	1:A:305:PRO:HG3	2.14	0.47
1:A:683:ILE:HG21	1:A:686:THR:HG23	1.97	0.47
1:A:702:MET:HA	1:A:715:ARG:O	2.14	0.47
1:A:270:ARG:HG2	1:A:297:TYR:CE2	2.49	0.47
1:A:487:LEU:HG	1:A:488:ILE:HD12	1.97	0.47
1:A:586:THR:HB	1:A:743:LEU:HD11	1.98	0.46
1:A:425:ILE:O	1:A:454:GLY:HA3	2.15	0.46
1:A:576:ASN:OD1	1:A:576:ASN:N	2.48	0.46
1:A:226:TYR:O	1:A:237:THR:HA	2.16	0.46
1:A:451:GLU:OE1	2:A:801:PEG:H22	2.15	0.46
1:A:286:ILE:O	1:A:287:PRO:C	2.57	0.45
1:A:455:MET:HE1	1:A:484:GLU:HB2	1.99	0.45
1:A:334:ALA:HA	1:A:360:TYR:O	2.16	0.45
1:A:398:HIS:O	1:A:399:LEU:HD12	2.17	0.45
1:A:651:ASP:O	1:A:670:ALA:HA	2.16	0.45
1:A:200:CYS:HB3	1:A:204:ILE:HD12	2.00	0.44
1:A:273:CYS:HB2	1:A:300:ARG:HB2	1.98	0.44
1:A:463:ILE:C	1:A:464:ILE:HD13	2.42	0.44
1:A:451:GLU:HA	1:A:474:GLU:O	2.18	0.44
1:A:370:LYS:HA	1:A:400:THR:O	2.18	0.44
1:A:594:LYS:HA	1:A:595:PRO:HD2	1.80	0.44
1:A:447:ARG:HA	1:A:447:ARG:HD2	1.60	0.43
1:A:342:SER:HA	1:A:368:ASN:HB3	2.00	0.43
1:A:417:SER:HA	1:A:446:HIS:O	2.18	0.43
1:A:591:TYR:HA	1:A:735:ILE:O	2.19	0.43
1:A:321:ALA:O	1:A:325:PRO:HA	2.19	0.43
1:A:524:TYR:CD2	1:A:527:GLN:HG3	2.54	0.43
1:A:241:THR:C	1:A:243:GLY:H	2.27	0.42
1:A:252:ALA:HB1	1:A:258:VAL:HG23	2.01	0.42
1:A:400:THR:HA	1:A:422:GLU:O	2.18	0.42
1:A:634:LEU:HD23	1:A:645:SER:OG	2.20	0.42
1:A:527:GLN:O	1:A:528:SER:C	2.61	0.42
1:A:417:SER:HB3	1:A:418:TYR:HD2	1.85	0.42
1:A:283:VAL:HG12	1:A:322:LYS:HG3	2.02	0.42
1:A:567:ARG:HD3	1:A:567:ARG:C	2.45	0.42
1:A:447:ARG:HD2	1:A:470:ALA:O	2.20	0.41
1:A:248:ALA:C	1:A:250:PHE:H	2.28	0.41
1:A:431:GLY:CA	1:A:439:ASN:OD1	2.60	0.41
1:A:291:ASN:OD1	1:A:291:ASN:N	2.49	0.41
1:A:406:ILE:HD13	1:A:407:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HZ2	1:A:191:LYS:HA	1.85	0.41
1:A:257:ASP:OD1	1:A:259:SER:HB2	2.21	0.41
1:A:491:ASN:OD1	1:A:492:ARG:N	2.52	0.41
1:A:624:ASN:HA	1:A:654:VAL:O	2.21	0.41
1:A:365:HIS:HA	1:A:395:ASN:O	2.21	0.40
1:A:469:SER:HA	1:A:506:SER:O	2.22	0.40
1:A:404:ARG:HG3	1:A:407:GLU:HG3	2.03	0.40
1:A:199:GLN:O	1:A:200:CYS:HB3	2.22	0.40
1:A:233:ASN:O	1:A:234:LEU:HD23	2.22	0.40
1:A:546:ILE:HD13	1:A:546:ILE:HG21	1.86	0.40
1:A:638:SER:HB3	1:A:731:THR:HG21	2.04	0.40
1:A:337:ASP:OD1	1:A:337:ASP:C	2.64	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	604/616 (98%)	541 (90%)	50 (8%)	13 (2%)	5 10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	187	LYS
1	A	718	PRO
1	A	167	GLN
1	A	242	THR
1	A	249	ARG
1	A	442	SER
1	A	200	CYS
1	A	291	ASN

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Mol	Chain	Res	Type
1	A	687	GLY
1	A	382	ARG
1	A	257	ASP
1	A	186	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	A	507/518 (98%)	456 (90%)	51 (10%)	7 15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	THR
1	A	173	ARG
1	A	174	LEU
1	A	180	THR
1	A	187	LYS
1	A	191	LYS
1	A	195	VAL
1	A	196	ILE
1	A	198	VAL
1	A	213	ARG
1	A	234	LEU
1	A	273	CYS
1	A	275	THR
1	A	320	SER
1	A	323	LEU
1	A	326	THR
1	A	327	SER
1	A	344	ILE
1	A	358	ARG
1	A	361	ASN
1	A	362	ILE
1	A	380	VAL

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Mol	Chain	Res	Type
1	A	384	VAL
1	A	391	SER
1	A	406	ILE
1	A	407	GLU
1	A	422	GLU
1	A	439	ASN
1	A	442	SER
1	A	447	ARG
1	A	451	GLU
1	A	456	LEU
1	A	464	ILE
1	A	501	SER
1	A	503	LEU
1	A	504	VAL
1	A	541	LYS
1	A	544	VAL
1	A	609	THR
1	A	617	THR
1	A	626	LYS
1	A	649	LYS
1	A	685	SER
1	A	686	THR
1	A	699	THR
1	A	702	MET
1	A	717	SER
1	A	721	ASN
1	A	723	SER
1	A	724	SER
1	A	744	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	295	ASN
1	A	361	ASN
1	A	363	ASN
1	A	395	ASN
1	A	440	ASN
1	A	632	ASN
1	A	642	ASN
1	A	747	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 ⓘ

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	$\# Z > 2$
2	PEG	A	801	-	6,6,6	1.15	0	5,5,5	0.78	0
2	PEG	A	802	-	6,6,6	0.69	0	5,5,5	0.33	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	PEG	A	801	-	-	2/4/4/4	-
2	PEG	A	802	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	PEG	O1-C1-C2-O2
2	A	801	PEG	O1-C1-C2-O2
2	A	801	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PEG	1	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	606/616 (98%)	-0.49	0 100 100	30, 56, 88, 118	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	PEG	A	802	7/7	0.81	0.16	45,63,74,74	0
2	PEG	A	801	7/7	0.83	0.17	47,68,89,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.