



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:21 PM UTC

PDB ID : 4RU5 / pdb_00004ru5
Title : Crystal Structure of the Pseudomonas phage phi297 tailspike gp61
Authors : Browning, C.; Sycheva, L.V.; Shneider, M.M.; Leiman, P.G.
Deposited on : 2014-11-18
Resolution : 1.52 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

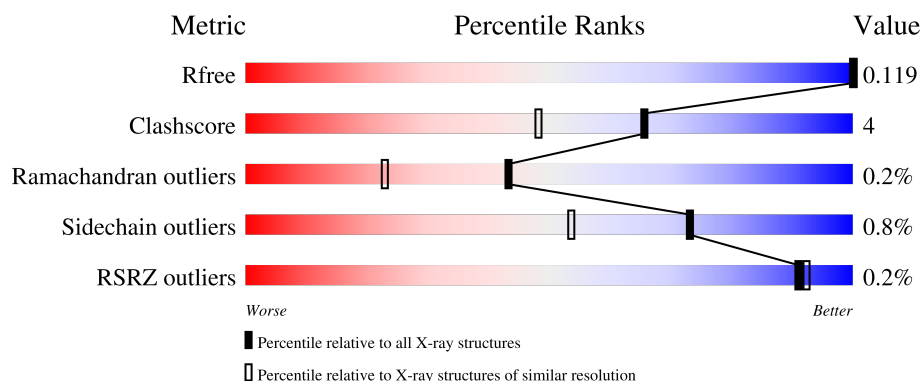
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	605	93% 6%
1	B	605	92% 8%
1	C	605	93% 6%

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
5	ACT	B	810	-	-	X	-
5	ACT	C	813	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17240 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 gp27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	21	0
			4644	2893	813	913	25			
1	B	600	Total	C	N	O	S	0	29	0
			4696	2925	821	925	25			
1	C	602	Total	C	N	O	S	0	22	0
			4671	2908	814	924	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	-	expression tag	UNP H2BD96
B	142	SER	-	expression tag	UNP H2BD96
C	142	SER	-	expression tag	UNP H2BD96

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

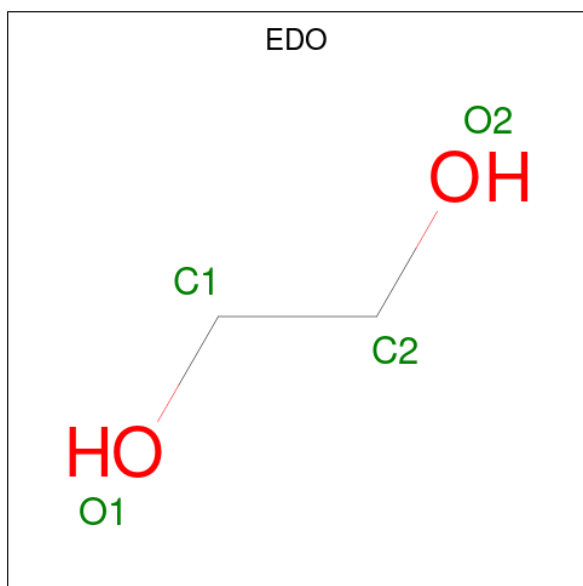
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Na	0	0
			6	6		
3	B	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Na	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



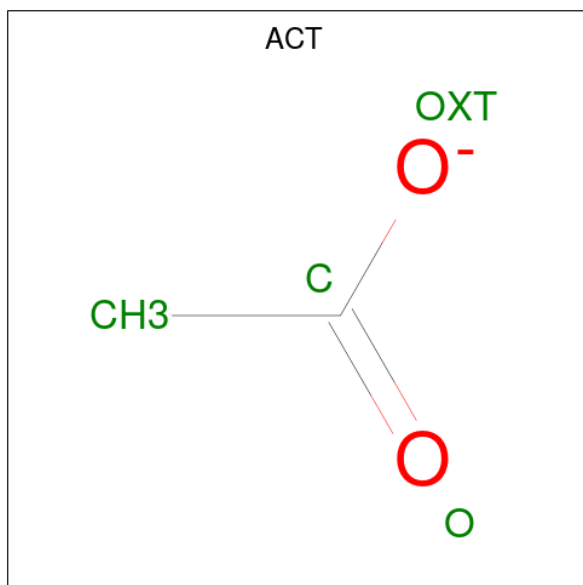
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

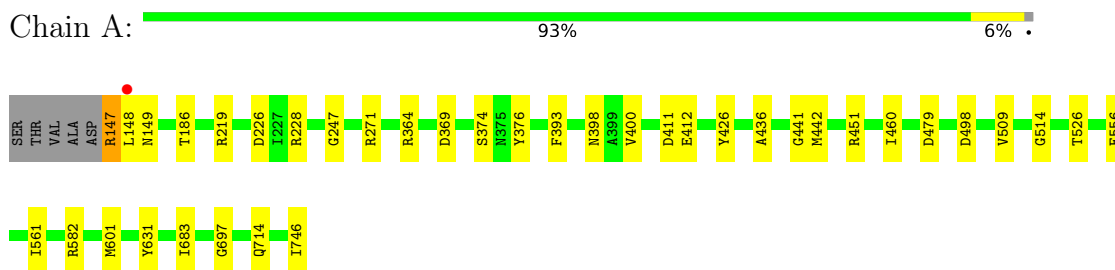
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1003	Total 1003	O 1003	0	0
6	B	1120	Total 1120	O 1120	0	0
6	C	1010	Total 1010	O 1010	0	0

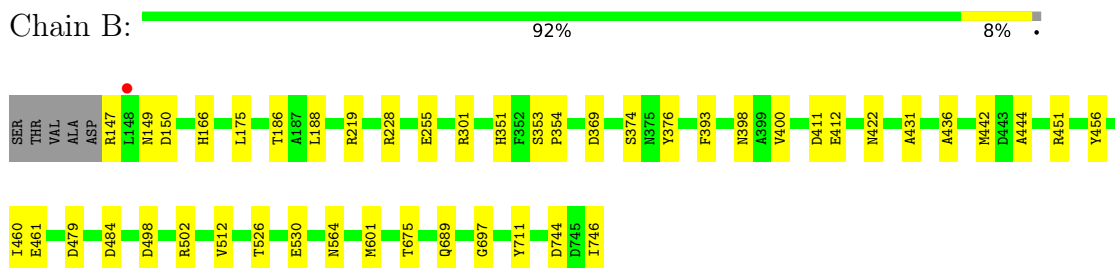
3 Residue-property plots

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.

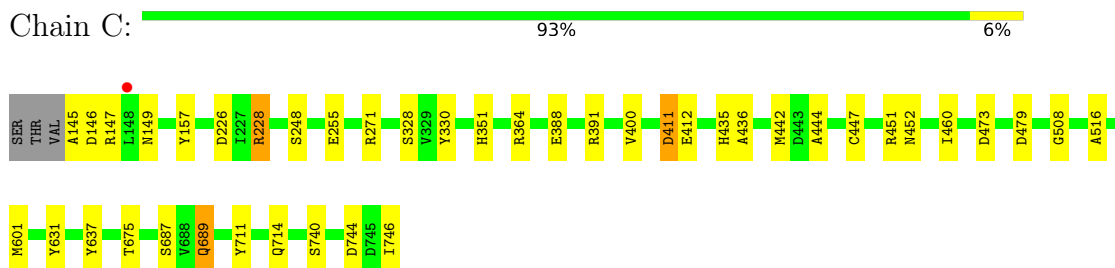
• Molecule 1: tailspike gp27



• Molecule 1: tailspike gp27



• Molecule 1: tailspike gp27



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.62Å 124.70Å 83.56Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	46.37 – 1.52 46.37 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.37-1.52) 98.2 (46.37-1.52)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.079 , 0.120 0.079 , 0.119	Depositor DCC
R_{free} test set	16066 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	17240	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: NA, ACT, CA, EDO

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	1.15	6/4746 (0.1%)	0.99	1/6472 (0.0%)
1	B	1.12	4/4798 (0.1%)	0.98	1/6542 (0.0%)
1	C	1.10	6/4773 (0.1%)	0.99	5/6509 (0.1%)
All	All	1.12	16/14317 (0.1%)	0.99	7/19523 (0.0%)

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	1
1	C	0	1
All	All	0	2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	ASP	C-O	8.33	1.34	1.24
1	C	228	ARG	CZ-NH1	7.50	1.43	1.32
1	A	714	GLN	CD-NE2	-6.00	1.20	1.33
1	C	271	ARG	CD-NE	-5.86	1.38	1.46
1	C	637	TYR	CE1-CZ	-5.70	1.24	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	CG-CD-NE	7.12	127.66	112.00
1	C	351	HIS	CA-CB-CG	5.33	119.13	113.80
1	C	452	ASN	CA-C-N	5.29	126.19	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	ASN	C-N-CA	5.29	126.19	122.33
1	C	364	ARG	NE-CZ-NH1	-5.24	116.26	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	631	TYR	Sidechain
1	C	631	TYR	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	4644	0	4447	28	0
1	B	4696	0	4499	41	0
1	C	4671	0	4462	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	16	0	22	0	0
4	B	12	0	15	4	0
4	C	24	0	33	2	0
5	A	4	0	3	1	0
5	B	12	0	9	4	0
5	C	12	0	9	5	0
6	A	1003	0	0	17	3
6	B	1120	0	0	26	1
6	C	1010	0	0	12	2
All	All	17240	0	13499	104	3

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.

The worst 5 of 104 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:601[B]:MET:HE2	6:A:1861:HOH:O	1.25	1.26
1:A:601[B]:MET:SD	6:A:1787:HOH:O	1.92	1.25
1:B:442[A]:MET:HE3	6:B:1904:HOH:O	1.07	1.23
1:B:601[B]:MET:SD	6:C:1455:HOH:O	1.97	1.20
1:B:675:THR:H	5:B:810:ACT:H3	1.08	1.17

All (3) 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)
6:A:1630:HOH:O	6:C:1779:HOH:O[4_757]	2.00	0.20
6:A:1518:HOH:O	6:B:1605:HOH:O[1_556]	2.04	0.16
6:A:1784:HOH:O	6:C:1741:HOH:O[4_757]	2.14	0.06

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	619/605 (102%)	595 (96%)	23 (4%)	1 (0%)	43	23
1	B	627/605 (104%)	603 (96%)	23 (4%)	1 (0%)	43	23
1	C	623/605 (103%)	597 (96%)	25 (4%)	1 (0%)	43	23
All	All	1869/1815 (103%)	1795 (96%)	71 (4%)	3 (0%)	43	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	ASP
1	B	411	ASP
1	C	411	ASP

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	495/478 (104%)	492 (99%)	3 (1%)	78	61
1	B	503/478 (105%)	499 (99%)	4 (1%)	73	53
1	C	498/478 (104%)	493 (99%)	5 (1%)	68	44
All	All	1496/1434 (104%)	1484 (99%)	12 (1%)	73	53

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	146	ASP
1	C	411	ASP
1	C	746	ILE
1	C	412	GLU
1	B	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	615	GLN
1	C	714	GLN
1	B	503	ASN
1	B	674	GLN
1	B	685	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

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	$\# Z > 2$
4	EDO	A	811	-	3,3,3	0.50	0	2,2,2	0.93	0
4	EDO	B	807	-	3,3,3	1.63	1 (33%)	2,2,2	0.53	0
5	ACT	C	813	-	3,3,3	0.85	0	3,3,3	1.52	1 (33%)
4	EDO	C	807	-	3,3,3	0.37	0	2,2,2	0.35	0
5	ACT	B	810	-	3,3,3	2.40	2 (66%)	3,3,3	1.38	0
5	ACT	C	811	-	3,3,3	1.27	0	3,3,3	0.76	0
4	EDO	B	806	-	3,3,3	0.99	0	2,2,2	0.64	0
4	EDO	A	810	-	3,3,3	0.63	0	2,2,2	1.23	0
4	EDO	A	812	-	3,3,3	1.30	0	2,2,2	0.64	0
5	ACT	B	809	-	3,3,3	1.59	1 (33%)	3,3,3	0.70	0
5	ACT	C	812	-	3,3,3	1.72	1 (33%)	3,3,3	0.48	0
4	EDO	A	809	-	3,3,3	1.76	1 (33%)	2,2,2	1.45	0
4	EDO	C	805	-	3,3,3	0.52	0	2,2,2	0.34	0
4	EDO	C	808	-	3,3,3	0.53	0	2,2,2	0.26	0
5	ACT	B	808	-	3,3,3	1.02	0	3,3,3	1.04	0
4	EDO	C	809	-	3,3,3	0.84	0	2,2,2	0.45	0
4	EDO	B	805	-	3,3,3	1.28	0	2,2,2	0.72	0
5	ACT	A	813	-	3,3,3	1.52	0	3,3,3	0.49	0
4	EDO	C	810	-	3,3,3	0.53	0	2,2,2	0.48	0
4	EDO	C	806	-	3,3,3	2.03	1 (33%)	2,2,2	0.58	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
4	EDO	A	811	-	-	0/1/1/1	-
4	EDO	C	809	-	-	1/1/1/1	-
4	EDO	B	805	-	-	0/1/1/1	-
4	EDO	A	809	-	-	1/1/1/1	-
4	EDO	B	806	-	-	1/1/1/1	-
4	EDO	B	807	-	-	1/1/1/1	-
4	EDO	A	810	-	-	0/1/1/1	-
4	EDO	C	805	-	-	0/1/1/1	-
4	EDO	C	810	-	-	0/1/1/1	-
4	EDO	A	812	-	-	0/1/1/1	-
4	EDO	C	807	-	-	1/1/1/1	-
4	EDO	C	806	-	-	0/1/1/1	-
4	EDO	C	808	-	-	1/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	812	ACT	O-C	2.98	1.35	1.22
5	B	810	ACT	OXT-C	-2.98	1.17	1.30
4	C	806	EDO	O1-C1	-2.91	1.27	1.42
4	B	807	EDO	O1-C1	-2.75	1.28	1.42
5	B	809	ACT	OXT-C	-2.54	1.19	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	813	ACT	O-C-CH3	-2.10	113.92	122.53

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	809	EDO	O1-C1-C2-O2
4	C	807	EDO	O1-C1-C2-O2
4	C	809	EDO	O1-C1-C2-O2
4	B	806	EDO	O1-C1-C2-O2
4	B	807	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	813	ACT	3	0
5	B	810	ACT	3	0
5	C	811	ACT	1	0
4	B	806	EDO	3	0
5	C	812	ACT	1	0
4	C	808	EDO	1	0
5	B	808	ACT	1	0
4	B	805	EDO	1	0
5	A	813	ACT	1	0
4	C	806	EDO	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	600/605 (99%)	-0.83	1 (0%) 91 92	5, 14, 23, 54	21 (3%)
1	B	600/605 (99%)	-0.86	1 (0%) 91 92	5, 13, 21, 76	29 (4%)
1	C	602/605 (99%)	-0.82	1 (0%) 91 92	5, 14, 27, 109	22 (3%)
All	All	1802/1815 (99%)	-0.83	3 (0%) 91 92	5, 14, 24, 109	72 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	LEU	3.6
1	A	148	LEU	2.8
1	C	148	LEU	2.1

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
4	EDO	A	812	4/4	0.85	0.14	40,41,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	807	4/4	0.91	0.13	36,43,47,82	0
4	EDO	C	808	4/4	0.92	0.09	38,43,57,76	0
3	NA	A	803	1/1	0.93	0.15	60,60,60,60	0
5	ACT	B	809	4/4	0.93	0.11	49,49,49,52	0
5	ACT	C	812	4/4	0.93	0.11	28,31,32,57	0
3	NA	A	808	1/1	0.94	0.14	55,55,55,55	0
5	ACT	C	811	4/4	0.94	0.09	25,31,33,37	0
3	NA	A	807	1/1	0.94	0.10	64,64,64,64	0
5	ACT	B	810	4/4	0.95	0.10	17,31,55,59	0
3	NA	A	804	1/1	0.95	0.20	58,58,58,58	0
3	NA	B	803	1/1	0.95	0.22	70,70,70,70	0
5	ACT	C	813	4/4	0.95	0.12	17,36,64,70	0
4	EDO	B	807	4/4	0.96	0.08	25,28,41,47	0
3	NA	C	804	1/1	0.96	0.12	50,50,50,50	0
4	EDO	A	810	4/4	0.96	0.09	21,27,36,42	0
3	NA	B	804	1/1	0.96	0.21	54,54,54,54	0
3	NA	A	806	1/1	0.97	0.13	44,44,44,44	0
3	NA	A	805	1/1	0.97	0.20	67,67,67,67	0
5	ACT	A	813	4/4	0.98	0.04	27,27,28,29	0
5	ACT	B	808	4/4	0.98	0.06	23,24,33,34	0
3	NA	C	803	1/1	0.98	0.07	38,38,38,38	0
4	EDO	C	806	4/4	0.98	0.07	21,21,23,26	0
4	EDO	A	811	4/4	0.98	0.06	17,32,34,38	0
4	EDO	A	809	4/4	0.98	0.05	19,24,32,33	0
4	EDO	C	810	4/4	0.98	0.07	23,40,41,44	0
4	EDO	B	806	4/4	0.99	0.05	17,23,30,39	0
4	EDO	B	805	4/4	0.99	0.05	20,20,25,29	0
4	EDO	C	805	4/4	0.99	0.04	17,18,19,24	0
4	EDO	C	809	4/4	0.99	0.05	19,28,29,34	0
2	CA	A	801	1/1	1.00	0.05	17,17,17,17	0
2	CA	A	802	1/1	1.00	0.05	18,18,18,18	0
2	CA	B	801	1/1	1.00	0.05	15,15,15,15	0
2	CA	B	802	1/1	1.00	0.06	17,17,17,17	0
2	CA	C	801	1/1	1.00	0.05	19,19,19,19	0
2	CA	C	802	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.