



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 11:32 AM EDT

PDB ID : 2VE8 / pdb_00002ve8
Title : Xray structure of FtsK gamma domain (P. aeruginosa)
Authors : Lowe, J.; Allen, M.A.; Sherratt, D.J.
Deposited on : 2007-10-17
Resolution : 1.40 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
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

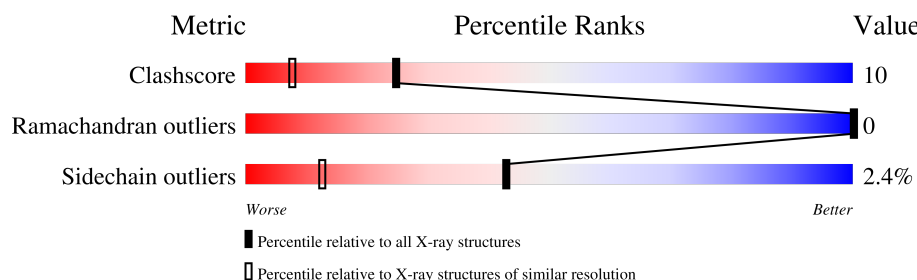
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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))
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	73	77% 14% • 8%
1	B	73	79% 10% 11%
1	C	73	71% 8% 5% • 14%
1	D	73	82% 7% • 7%
1	E	73	77% 12% • 8%
1	F	73	71% 16% • 10%
1	G	73	68% 12% • 16%
1	H	73	67% 18% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4633 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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			520	318	97	101	4			
1	B	65	Total	C	N	O	S	0	0	0
			500	308	92	96	4			
1	C	63	Total	C	N	O	S	0	0	1
			477	295	89	89	4			
1	D	68	Total	C	N	O	S	0	0	0
			526	321	98	103	4			
1	E	67	Total	C	N	O	S	0	0	1
			507	311	94	98	4			
1	F	66	Total	C	N	O	S	0	0	1
			500	306	93	97	4			
1	G	61	Total	C	N	O	S	0	0	1
			465	286	88	87	4			
1	H	63	Total	C	N	O	S	0	0	1
			477	294	90	89	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	92	Total	O	0	0
			92	92		
2	C	89	Total	O	0	0
			89	89		
2	D	81	Total	O	0	0
			81	81		
2	E	67	Total	O	0	0
			67	67		
2	F	67	Total	O	0	0
			67	67		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	97	Total 97	O 97	0	0
2	H	74	Total 74	O 74	0	0

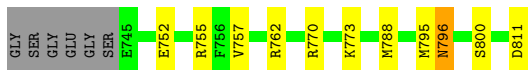
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: DNA TRANSLOCASE FTSK

Chain A: 



- Molecule 1: DNA TRANSLOCASE FTSK

Chain B: 



- Molecule 1: DNA TRANSLOCASE FTSK

Chain C: 



- Molecule 1: DNA TRANSLOCASE FTSK

Chain D: 



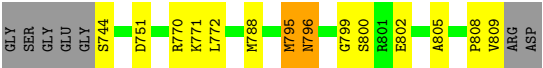
- Molecule 1: DNA TRANSLOCASE FTSK

Chain E: 

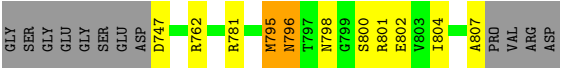


- Molecule 1: DNA TRANSLOCASE FTSK

Chain F: 



● Molecule 1: DNA TRANSLOCASE FTSK



● Molecule 1: DNA TRANSLOCASE FTSK



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.49Å 58.50Å 95.41Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	95.35 – 1.40	Depositor
% Data completeness (in resolution range)	99.8 (95.35-1.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.144 , 0.192	Depositor
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4633	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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 ⓘ

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	1.52	2/526 (0.4%)	1.42	1/708 (0.1%)
1	B	1.63	0/506	1.29	0/683
1	C	1.66	5/482 (1.0%)	1.30	1/649 (0.2%)
1	D	1.55	2/532 (0.4%)	1.28	2/716 (0.3%)
1	E	1.66	4/513 (0.8%)	1.32	0/693
1	F	1.75	5/506 (1.0%)	1.51	6/683 (0.9%)
1	G	1.76	8/470 (1.7%)	1.46	1/633 (0.2%)
1	H	1.60	3/483 (0.6%)	1.30	1/652 (0.2%)
All	All	1.64	29/4018 (0.7%)	1.36	12/5417 (0.2%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	795	MET	SD-CE	-7.40	1.61	1.79
1	G	762	ARG	CZ-NH1	7.35	1.43	1.32
1	F	802	GLU	CG-CD	7.06	1.69	1.52
1	F	805	ALA	C-N	6.89	1.42	1.33
1	C	795	MET	CB-CG	6.77	1.72	1.52
1	E	806	PRO	C-O	6.62	1.31	1.23
1	G	762	ARG	CZ-NH2	6.49	1.41	1.33
1	H	768	VAL	N-CA	6.40	1.54	1.46
1	E	809	VAL	C-N	-6.37	1.24	1.33
1	G	804	ILE	C-O	-6.36	1.16	1.23
1	C	746	ASP	CB-CG	6.10	1.67	1.52
1	A	757	VAL	CB-CG2	-6.09	1.32	1.52
1	G	804	ILE	CA-CB	6.07	1.63	1.54
1	G	801	ARG	CZ-NH1	6.00	1.41	1.32
1	G	802	GLU	CD-OE1	5.92	1.36	1.25
1	G	802	GLU	CG-CD	5.84	1.66	1.52
1	F	805	ALA	CA-C	5.66	1.59	1.53
1	F	795	MET	SD-CE	-5.54	1.65	1.79
1	F	808	PRO	C-N	-5.50	1.25	1.33
1	C	799	GLY	N-CA	5.45	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	809	VAL	C-N	-5.42	1.25	1.33
1	C	800	SER	C-O	-5.38	1.17	1.23
1	E	802	GLU	CG-CD	5.37	1.65	1.52
1	H	808	PRO	C-N	-5.26	1.25	1.33
1	D	788	MET	C-O	5.15	1.30	1.24
1	A	795	MET	CB-CG	-5.06	1.37	1.52
1	D	784	GLU	N-CA	5.05	1.52	1.46
1	H	798	ASN	CA-CB	-5.05	1.45	1.53
1	E	778	ARG	CD-NE	-5.03	1.39	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	770	ARG	NE-CZ-NH2	7.65	126.09	119.20
1	F	805	ALA	O-C-N	6.66	128.88	121.43
1	F	805	ALA	CA-C-N	-6.58	113.20	119.85
1	F	805	ALA	C-N-CA	-6.58	113.20	119.85
1	D	746	ASP	CA-CB-CG	-6.33	106.27	112.60
1	A	755	ARG	CG-CD-NE	-5.81	99.21	112.00
1	F	751	ASP	CB-CG-OD2	5.72	131.57	118.40
1	F	770	ARG	NE-CZ-NH1	-5.49	116.02	121.50
1	G	802	GLU	CB-CG-CD	5.23	121.50	112.60
1	C	757	VAL	CG1-CB-CG2	5.16	122.15	110.80
1	D	781	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	H	804	ILE	CB-CA-C	-5.04	105.59	111.94

There are no chirality outliers.

There are no planarity outliers.

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	520	0	522	11	0
1	B	500	0	505	7	0
1	C	477	0	485	15	1
1	D	526	0	527	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	507	0	510	9	0
1	F	500	0	501	11	0
1	G	465	0	474	9	0
1	H	477	0	486	14	1
2	A	94	0	0	4	0
2	B	92	0	0	5	0
2	C	89	0	0	10	0
2	D	81	0	0	6	0
2	E	67	0	0	3	0
2	F	67	0	0	3	0
2	G	97	0	0	4	0
2	H	74	0	0	5	0
All	All	4633	0	4010	78	1

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 (78) 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:B:809:VAL:C	2:B:2092:HOH:O	1.72	1.30
1:D:744:SER:HB2	2:D:2001:HOH:O	1.15	1.29
1:H:802:GLU:CD	2:H:2063:HOH:O	1.76	1.25
1:H:802:GLU:OE2	2:H:2062:HOH:O	1.60	1.18
1:H:802:GLU:OE1	2:H:2063:HOH:O	1.63	1.12
1:B:752:GLU:HB2	1:C:752:GLU:OE1	1.54	1.07
1:D:752:GLU:OE1	2:D:2021:HOH:O	1.73	1.07
1:H:802:GLU:OE2	2:H:2063:HOH:O	1.68	1.06
1:F:744:SER:N	2:F:2002:HOH:O	1.85	1.06
1:E:744:SER:N	2:E:2001:HOH:O	1.98	0.95
1:C:796:ASN:HB3	2:C:2064:HOH:O	1.65	0.94
1:C:746:ASP:N	2:C:2006:HOH:O	2.06	0.89
1:G:747:ASP:N	2:G:2005:HOH:O	2.06	0.87
1:C:795:MET:HE2	1:C:799:GLY:O	1.74	0.87
1:C:796:ASN:C	1:C:796:ASN:HD22	1.88	0.79
1:C:800:SER:HB2	2:C:2070:HOH:O	1.81	0.79
1:H:747:ASP:N	2:H:2001:HOH:O	2.17	0.77
1:F:809:VAL:N	2:F:2066:HOH:O	2.18	0.76
1:A:770:ARG:NH2	2:A:2047:HOH:O	2.19	0.75
1:C:795:MET:SD	2:C:2089:HOH:O	2.45	0.74
1:D:781:ARG:HD2	2:D:2047:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:LYS:NZ	2:B:2046:HOH:O	2.22	0.71
1:A:752:GLU:HB2	1:D:752:GLU:OE2	1.91	0.70
1:D:744:SER:CB	2:D:2001:HOH:O	1.96	0.68
1:E:796:ASN:C	1:E:796:ASN:HD22	2.05	0.63
1:H:796:ASN:C	1:H:796:ASN:HD22	2.05	0.63
1:E:771:LYS:HG3	1:E:772:LEU:HD22	1.80	0.63
1:F:795:MET:HG2	1:F:799:GLY:HA2	1.81	0.62
1:H:749:LEU:HB2	1:H:782:MET:HE1	1.81	0.61
1:F:795:MET:HE3	1:H:795:MET:SD	2.40	0.61
1:A:796:ASN:ND2	1:A:800:SER:H	1.98	0.60
1:G:796:ASN:C	1:G:796:ASN:HD22	2.10	0.59
1:B:762:ARG:HD3	2:B:2033:HOH:O	2.03	0.58
1:F:788:MET:SD	2:F:2016:HOH:O	2.57	0.58
1:A:811:ASP:OD1	1:A:811:ASP:C	2.47	0.56
1:D:796:ASN:C	1:D:796:ASN:HD22	2.14	0.56
1:F:796:ASN:HD22	1:F:796:ASN:C	2.12	0.56
1:C:800:SER:CB	2:C:2070:HOH:O	2.49	0.54
1:F:795:MET:HE3	1:H:795:MET:HE3	1.91	0.53
1:A:796:ASN:C	1:A:796:ASN:HD22	2.17	0.52
1:E:771:LYS:CG	1:E:772:LEU:HD22	2.40	0.52
1:F:771:LYS:HG3	1:F:772:LEU:HD22	1.91	0.52
1:G:781:ARG:NH1	2:G:2059:HOH:O	2.44	0.50
1:A:762:ARG:NE	2:A:2038:HOH:O	2.44	0.49
1:C:796:ASN:C	1:C:796:ASN:ND2	2.65	0.49
1:E:809:VAL:HG23	1:E:810:ARG:N	2.28	0.49
1:D:781:ARG:NH2	2:D:2047:HOH:O	2.10	0.48
1:C:795:MET:CB	2:C:2089:HOH:O	2.61	0.48
1:A:811:ASP:OXT	1:C:755:ARG:NH1	2.38	0.48
1:B:745:GLU:CA	2:B:2005:HOH:O	2.62	0.47
1:C:795:MET:HB2	2:C:2089:HOH:O	2.14	0.47
1:F:795:MET:CE	1:H:795:MET:HE3	2.45	0.47
1:D:752:GLU:CD	2:D:2021:HOH:O	2.41	0.47
1:C:770:ARG:NH2	2:C:2038:HOH:O	2.07	0.46
1:C:795:MET:CG	2:C:2089:HOH:O	2.64	0.46
1:G:795:MET:HE3	1:G:795:MET:HB3	1.58	0.46
1:G:796:ASN:ND2	1:G:800:SER:H	2.14	0.45
1:H:796:ASN:ND2	1:H:800:SER:H	2.15	0.45
1:E:784:GLU:HG3	2:E:2046:HOH:O	2.17	0.45
1:A:773:LYS:NZ	2:A:2050:HOH:O	2.09	0.45
1:H:771:LYS:HG3	1:H:772:LEU:HD12	1.99	0.45
1:G:747:ASP:N	2:G:2008:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:796:ASN:C	1:H:796:ASN:ND2	2.73	0.44
1:A:788:MET:HE2	1:A:788:MET:HB3	1.72	0.44
1:G:807:ALA:N	2:G:2090:HOH:O	2.49	0.44
1:G:796:ASN:C	1:G:796:ASN:ND2	2.74	0.44
1:F:795:MET:HE3	1:H:795:MET:CE	2.48	0.44
1:A:796:ASN:ND2	1:A:796:ASN:C	2.77	0.43
1:F:796:ASN:ND2	1:F:800:SER:H	2.17	0.42
1:C:796:ASN:C	2:C:2065:HOH:O	2.61	0.42
1:B:745:GLU:N	2:B:2005:HOH:O	2.53	0.41
1:E:796:ASN:ND2	1:E:800:SER:H	2.18	0.41
1:B:755:ARG:O	1:B:759:GLU:HG3	2.21	0.41
1:D:796:ASN:C	1:D:796:ASN:ND2	2.79	0.41
1:E:744:SER:CA	2:E:2001:HOH:O	2.58	0.41
1:E:796:ASN:C	1:E:796:ASN:ND2	2.72	0.41
1:A:762:ARG:HB2	2:A:2038:HOH:O	2.21	0.41
1:G:796:ASN:ND2	1:G:798:ASN:H	2.19	0.40

All (1) 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)
1:C:802:GLU:OE1	1:H:748:PRO:CB[1_655]	2.03	0.17

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	65/73 (89%)	65 (100%)	0	0	100	100
1	B	63/73 (86%)	63 (100%)	0	0	100	100
1	C	59/73 (81%)	59 (100%)	0	0	100	100
1	D	66/73 (90%)	66 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	65/73 (89%)	65 (100%)	0	0	100	100
1	F	64/73 (88%)	63 (98%)	1 (2%)	0	100	100
1	G	59/73 (81%)	59 (100%)	0	0	100	100
1	H	61/73 (84%)	60 (98%)	1 (2%)	0	100	100
All	All	502/584 (86%)	500 (100%)	2 (0%)	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	55/58 (95%)	54 (98%)	1 (2%)	51	20
1	B	53/58 (91%)	53 (100%)	0	100	100
1	C	50/58 (86%)	48 (96%)	2 (4%)	28	5
1	D	56/58 (97%)	53 (95%)	3 (5%)	20	2
1	E	54/58 (93%)	53 (98%)	1 (2%)	50	18
1	F	53/58 (91%)	52 (98%)	1 (2%)	50	18
1	G	49/58 (84%)	48 (98%)	1 (2%)	48	17
1	H	50/58 (86%)	49 (98%)	1 (2%)	48	17
All	All	420/464 (90%)	410 (98%)	10 (2%)	43	12

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	796	ASN
1	C	795	MET
1	C	796	ASN
1	D	744	SER
1	D	770	ARG
1	D	796	ASN

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Mol	Chain	Res	Type
1	E	796	ASN
1	F	796	ASN
1	G	796	ASN
1	H	796	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	777	ASN
1	A	796	ASN
1	C	777	ASN
1	C	796	ASN
1	D	777	ASN
1	D	796	ASN
1	E	769	GLN
1	E	777	ASN
1	E	796	ASN
1	F	769	GLN
1	F	777	ASN
1	F	796	ASN
1	G	796	ASN
1	G	798	ASN
1	H	796	ASN
1	H	798	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.