



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:58 PM UTC

PDB ID : 7DFM / pdb\_00007dfm  
Title : Crystal structure of glycoside hydrolase family 11 beta-xylanase from *Streptomyces olivaceoviridis* E-86  
Authors : Fujimoto, Z.; Kishine, N.; Kaneko, S.  
Deposited on : 2020-11-09  
Resolution : 2.40 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](mailto: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 : 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

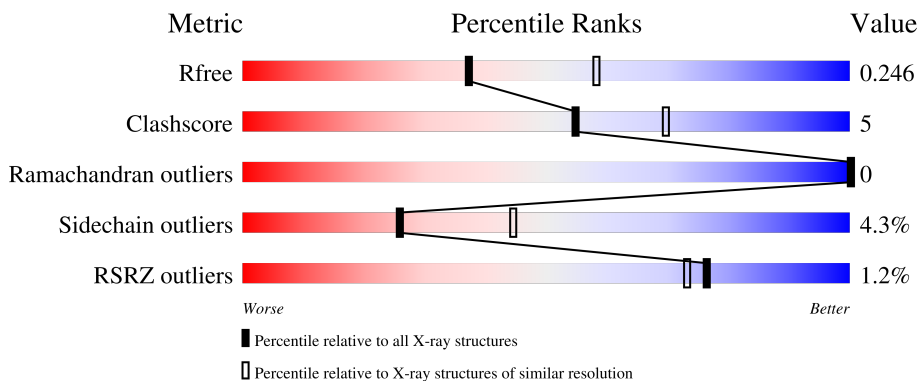
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	205	 79% 15% 5%
1	B	205	 80% 14% 6%
1	C	205	 78% 16% 6%
1	D	205	 75% 18% 5%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6144 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1499	942	253	300	4	0	0	0
1	B	193	1494	939	252	299	4	0	0	0
1	C	193	1494	939	252	299	4	0	0	0
1	D	194	1499	942	253	300	4	0	0	0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Cl	0	0
			7	7		
2	B	4	Total	Cl	0	0
			4	4		
2	C	6	Total	Cl	0	0
			6	6		
2	D	5	Total	Cl	0	0
			5	5		

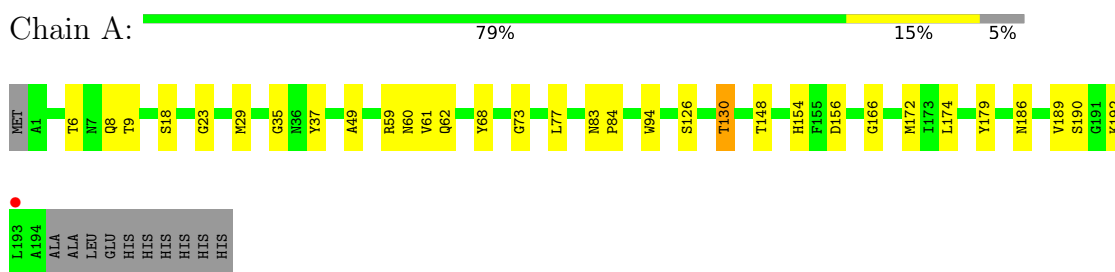
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	37	Total	O	0	0
			37	37		
3	C	28	Total	O	0	0
			28	28		
3	D	34	Total	O	0	0
			34	34		

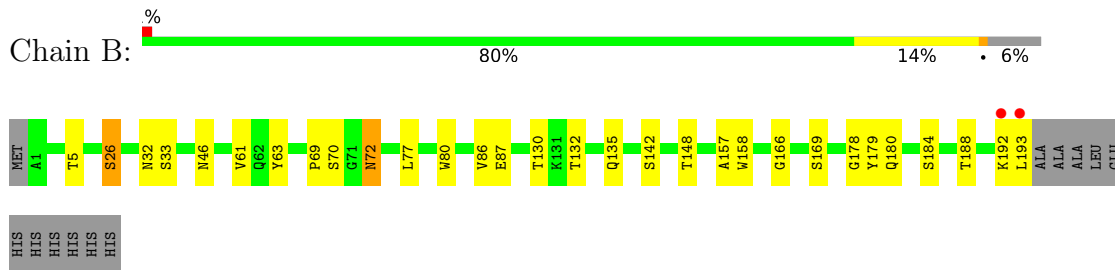
### 3 Residue-property plots [i](#)

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.

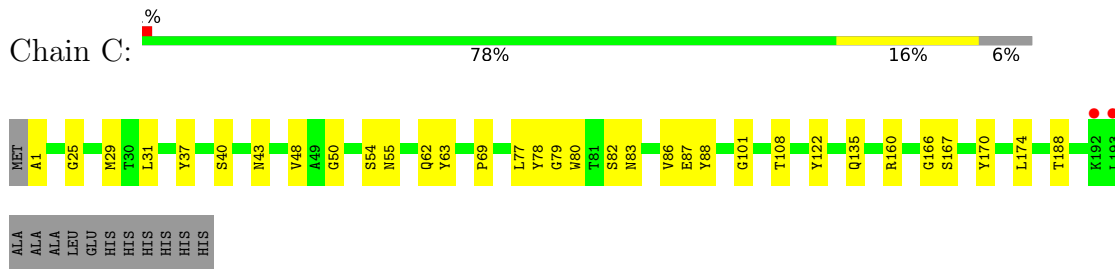
- Molecule 1: Endo-1,4-beta-xylanase



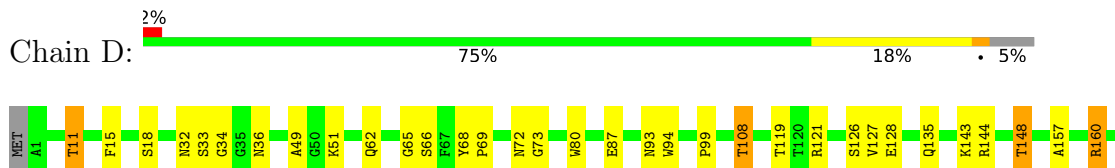
- Molecule 1: Endo-1,4-beta-xylanase



- Molecule 1: Endo-1,4-beta-xylanase



- Molecule 1: Endo-1,4-beta-xylanase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.04Å 135.04Å 72.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.41 – 2.40 49.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.41-2.40) 100.0 (49.41-2.40)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.168 , 0.245 0.175 , 0.246	Depositor DCC
$R_{free}$ test set	1571 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	1.17	3/1543 (0.2%)	1.45	6/2102 (0.3%)
1	B	1.09	2/1538 (0.1%)	1.45	8/2095 (0.4%)
1	C	1.16	1/1538 (0.1%)	1.48	3/2095 (0.1%)
1	D	1.17	1/1543 (0.1%)	1.49	6/2102 (0.3%)
All	All	1.15	7/6162 (0.1%)	1.47	23/8394 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	PRO	C-O	-6.41	1.16	1.23
1	C	69	PRO	C-O	-6.28	1.17	1.23
1	B	70	SER	C-O	6.08	1.31	1.23
1	B	166	GLY	C-O	5.73	1.29	1.23
1	A	60	ASN	C-O	5.37	1.30	1.23
1	A	154	HIS	CE1-NE2	5.10	1.37	1.32
1	A	179	TYR	C-O	5.05	1.29	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	GLY	CA-C-O	-10.38	115.47	122.22
1	B	132	THR	CA-CB-OG1	-7.05	99.02	109.60
1	D	11	THR	CA-CB-OG1	-6.61	99.68	109.60
1	C	122	TYR	CB-CA-C	6.13	120.12	110.19
1	B	72	ASN	CA-CB-CG	-5.95	106.65	112.60
1	A	130	THR	CA-CB-OG1	-5.95	100.67	109.60
1	B	130	THR	CA-CB-OG1	-5.95	100.67	109.60
1	B	32	ASN	CA-C-O	-5.75	115.01	121.40
1	B	26	SER	CB-CA-C	5.72	118.95	110.14
1	C	101	GLY	CA-C-O	-5.70	116.54	121.04

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	ARG	CA-C-O	-5.68	113.69	120.10
1	B	69	PRO	CA-C-O	-5.67	114.94	121.86
1	D	99	PRO	N-CA-CB	5.62	108.31	103.31
1	D	148	THR	CB-CA-C	5.49	119.25	109.38
1	D	108	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	156	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	32	ASN	CA-C-N	5.36	128.70	120.82
1	B	32	ASN	C-N-CA	5.36	128.70	120.82
1	A	190	SER	CA-C-O	-5.16	115.89	121.36
1	A	23	GLY	CA-C-N	5.10	124.82	119.92
1	A	23	GLY	C-N-CA	5.10	124.82	119.92
1	C	83	ASN	CB-CA-C	5.08	115.42	111.00
1	A	9	THR	CA-C-O	-5.02	115.76	121.68

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	1499	0	1371	13	0
1	B	1494	0	1366	11	0
1	C	1494	0	1366	18	0
1	D	1499	0	1371	21	0
2	A	7	0	0	0	0
2	B	4	0	0	0	0
2	C	6	0	0	0	0
2	D	5	0	0	0	0
3	A	37	0	0	0	0
3	B	37	0	0	0	0
3	C	28	0	0	0	0
3	D	34	0	0	0	0
All	All	6144	0	5474	55	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 (55) 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:29:MET:HE3	1:A:37:TYR:CD1	2.28	0.68
1:B:63:TYR:HA	1:B:188:THR:O	1.96	0.65
1:A:68:TYR:CD1	1:D:119:THR:HB	2.33	0.64
1:A:6:THR:O	1:A:8:GLN:HG2	1.99	0.63
1:C:79:GLY:HA3	1:C:88:TYR:CZ	2.35	0.61
1:C:80:TRP:HA	1:C:86:VAL:O	1.99	0.60
1:B:5:THR:H	1:C:55:ASN:ND2	1.98	0.60
1:C:160:ARG:HD2	1:D:126:SER:O	2.02	0.58
1:D:34:GLY:O	1:D:51:LYS:NZ	2.35	0.58
1:C:29:MET:HE2	1:C:37:TYR:CD2	2.42	0.55
1:C:108:THR:O	1:D:128:GLU:OE2	2.25	0.55
1:B:77:LEU:HD13	1:B:77:LEU:C	2.32	0.54
1:C:29:MET:HE1	1:C:50:GLY:CA	2.38	0.53
1:C:29:MET:CE	1:C:37:TYR:CD2	2.93	0.51
1:B:157:ALA:O	1:B:158:TRP:C	2.56	0.49
1:B:61:VAL:O	1:B:148:THR:HA	2.14	0.48
1:B:72:ASN:HD22	1:B:179:TYR:HB3	1.78	0.48
1:D:62:GLN:NE2	1:D:148:THR:OG1	2.44	0.47
1:C:55:ASN:HA	1:C:170:TYR:O	2.15	0.47
1:C:29:MET:HE1	1:C:50:GLY:N	2.30	0.46
1:B:80:TRP:CZ3	1:B:87:GLU:HB2	2.51	0.46
1:D:87:GLU:O	1:D:135:GLN:HA	2.15	0.46
1:D:94:TRP:CE2	1:D:143:LYS:HE2	2.51	0.46
1:C:87:GLU:O	1:C:135:GLN:HA	2.15	0.46
1:A:68:TYR:CE1	1:D:119:THR:HB	2.51	0.46
1:C:82:SER:O	1:C:166:GLY:HA3	2.15	0.46
1:B:80:TRP:HA	1:B:86:VAL:O	2.16	0.46
1:C:160:ARG:CD	1:D:126:SER:O	2.65	0.45
1:D:94:TRP:NE1	1:D:143:LYS:HE2	2.31	0.45
1:B:46:ASN:HA	1:B:178:GLY:O	2.17	0.45
1:B:87:GLU:O	1:B:135:GLN:HA	2.16	0.45
1:C:48:VAL:HG11	1:C:78:TYR:CE2	2.51	0.45
1:D:66:SER:HB2	1:D:68:TYR:CE2	2.51	0.45
1:A:61:VAL:O	1:A:148:THR:HA	2.18	0.44
1:A:186:ASN:HD21	1:D:72:ASN:ND2	2.14	0.44
1:D:80:TRP:NE1	1:D:127:VAL:HG13	2.33	0.44
1:A:73:GLY:O	1:A:94:TRP:HA	2.18	0.43
1:A:84:PRO:HD2	1:A:166:GLY:CA	2.48	0.43
1:A:77:LEU:HD11	1:A:172:MET:SD	2.58	0.43
1:D:73:GLY:O	1:D:94:TRP:HA	2.18	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:GLY:HA3	1:C:43:ASN:O	2.19	0.43
1:C:29:MET:HE2	1:C:37:TYR:CG	2.54	0.42
1:D:93:ASN:HB2	1:D:144:ARG:O	2.19	0.42
1:D:65:GLY:HA3	1:D:186:ASN:O	2.19	0.42
1:D:32:ASN:HB3	1:D:36:ASN:HB3	2.01	0.42
1:B:179:TYR:O	1:B:180:GLN:C	2.62	0.42
1:D:11:THR:HA	1:D:15:PHE:O	2.20	0.42
1:D:157:ALA:HA	1:D:160:ARG:HD3	2.00	0.42
1:D:18:SER:O	1:D:49:ALA:HA	2.19	0.42
1:A:59:ARG:HG2	1:A:172:MET:HE1	2.02	0.41
1:C:63:TYR:HA	1:C:188:THR:O	2.19	0.41
1:A:35:GLY:HA3	1:A:189:VAL:O	2.21	0.41
1:A:18:SER:O	1:A:49:ALA:HA	2.21	0.41
1:A:186:ASN:HD21	1:D:72:ASN:HD21	1.69	0.40
1:C:1:ALA:HA	1:C:31:LEU: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	192/205 (94%)	187 (97%)	5 (3%)	0	100	100
1	B	191/205 (93%)	186 (97%)	5 (3%)	0	100	100
1	C	191/205 (93%)	183 (96%)	8 (4%)	0	100	100
1	D	192/205 (94%)	188 (98%)	4 (2%)	0	100	100
All	All	766/820 (93%)	744 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	156/165 (94%)	150 (96%)	6 (4%)	29	49
1	B	156/165 (94%)	149 (96%)	7 (4%)	24	42
1	C	156/165 (94%)	150 (96%)	6 (4%)	29	49
1	D	156/165 (94%)	148 (95%)	8 (5%)	21	37
All	All	624/660 (94%)	597 (96%)	27 (4%)	26	44

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	83	ASN
1	A	126	SER
1	A	130	THR
1	A	174	LEU
1	A	192	LYS
1	B	26	SER
1	B	33	SER
1	B	142	SER
1	B	169	SER
1	B	184	SER
1	B	192	LYS
1	B	193	LEU
1	C	40	SER
1	C	54	SER
1	C	62	GLN
1	C	77	LEU
1	C	167	SER
1	C	174	LEU
1	D	33	SER
1	D	108	THR
1	D	121	ARG
1	D	167	SER
1	D	174	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	177	GLU
1	D	184	SER
1	D	189	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	46	ASN
1	A	118	GLN
1	B	83	ASN
1	C	46	ASN
1	C	55	ASN
1	C	83	ASN
1	C	96	ASN
1	C	141	GLN
1	D	60	ASN
1	D	62	GLN
1	D	72	ASN
1	D	83	ASN
1	D	141	GLN
1	D	180	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	194/205 (94%)	-0.51	1 (0%) 87 85	18, 26, 43, 71	0
1	B	193/205 (94%)	-0.40	2 (1%) 79 76	20, 28, 42, 84	0
1	C	193/205 (94%)	-0.38	2 (1%) 79 76	17, 27, 43, 70	0
1	D	194/205 (94%)	-0.32	4 (2%) 63 59	22, 29, 42, 84	0
All	All	774/820 (94%)	-0.40	9 (1%) 76 73	17, 28, 43, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	LEU	4.0
1	D	192	LYS	3.5
1	B	192	LYS	3.4
1	A	193	LEU	3.3
1	D	191	GLY	3.1
1	C	193	LEU	3.0
1	D	193	LEU	3.0
1	D	194	ALA	3.0
1	C	192	LYS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CL	D	301	1/1	0.94	0.07	39,39,39,39	0
2	CL	A	405	1/1	0.95	0.21	44,44,44,44	0
2	CL	D	304	1/1	0.95	0.06	41,41,41,41	0
2	CL	A	404	1/1	0.96	0.10	39,39,39,39	0
2	CL	D	305	1/1	0.96	0.06	41,41,41,41	0
2	CL	C	406	1/1	0.97	0.06	38,38,38,38	0
2	CL	B	403	1/1	0.97	0.04	33,33,33,33	0
2	CL	D	302	1/1	0.97	0.12	39,39,39,39	0
2	CL	C	403	1/1	0.97	0.07	43,43,43,43	0
2	CL	C	404	1/1	0.97	0.06	42,42,42,42	0
2	CL	B	401	1/1	0.98	0.04	34,34,34,34	0
2	CL	A	401	1/1	0.98	0.03	26,26,26,26	0
2	CL	B	404	1/1	0.98	0.07	38,38,38,38	0
2	CL	C	401	1/1	0.98	0.07	29,29,29,29	0
2	CL	D	303	1/1	0.98	0.07	42,42,42,42	0
2	CL	C	402	1/1	0.98	0.04	29,29,29,29	0
2	CL	A	407	1/1	0.98	0.05	29,29,29,29	0
2	CL	B	402	1/1	0.99	0.08	32,32,32,32	0
2	CL	A	406	1/1	0.99	0.08	28,28,28,28	0
2	CL	A	402	1/1	0.99	0.07	25,25,25,25	0
2	CL	C	405	1/1	0.99	0.06	36,36,36,36	0
2	CL	A	403	1/1	0.99	0.07	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.