wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 08:40 pm GMT

PDB ID	:	2XLB
Title	:	Acetyl xylan esterase from Bacillus pumilus without ligands
Authors	:	Gil-Ortiz, F.; Montoro-Garcia, S.; Polo, L.M.; Rubio, V.; Sanchez-Ferrer, A.
Deposited on	:	2010-07-20
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

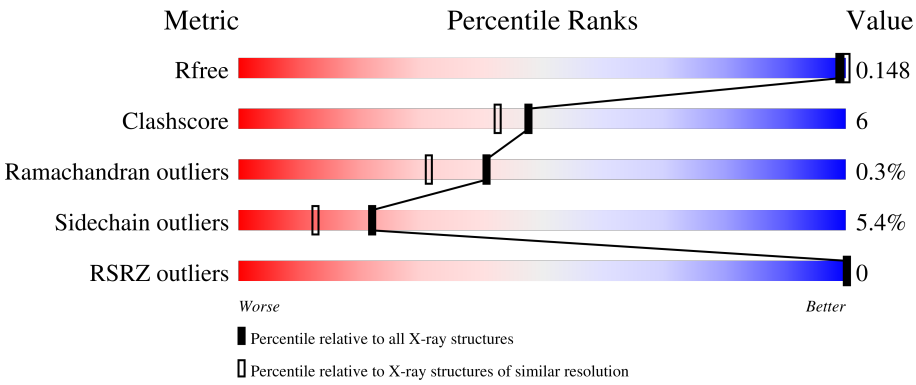
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	320	84% 13% • •
1	B	320	86% 12% • •
1	C	320	87% 11% • •
1	D	320	87% 11% • •
1	E	320	87% 10% • • •

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Mol	Chain	Length	Quality of chain
1	F	320	84% 13%
1	G	320	86% 12%
1	H	320	87% 11%
1	I	320	85% 13%
1	J	320	85% 12%
1	K	320	84% 12%
1	L	320	84% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31554 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 ACETYL XYLAN ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2512	1627	410	472	3	0	0	0
1	B	317	2512	1629	412	468	3	0	0	0
1	C	317	2504	1623	410	468	3	0	0	0
1	D	317	2504	1623	410	468	3	0	0	0
1	E	317	2501	1622	410	466	3	0	0	0
1	F	317	2504	1623	410	468	3	0	0	0
1	G	317	2504	1623	410	468	3	0	0	0
1	H	317	2501	1622	410	466	3	0	0	0
1	I	317	2501	1622	410	466	3	0	0	0
1	J	317	2501	1622	410	466	3	0	0	0
1	K	317	2501	1622	410	466	3	0	0	0
1	L	317	2505	1624	410	468	3	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASP	GLY	conflict	UNP Q9K5F2
A	236	GLU	LYS	conflict	UNP Q9K5F2
A	270	GLN	LYS	conflict	UNP Q9K5F2
A	289	GLU	ASP	conflict	UNP Q9K5F2
B	97	ASP	GLY	conflict	UNP Q9K5F2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	236	GLU	LYS	conflict	UNP Q9K5F2
B	270	GLN	LYS	conflict	UNP Q9K5F2
B	289	GLU	ASP	conflict	UNP Q9K5F2
C	97	ASP	GLY	conflict	UNP Q9K5F2
C	236	GLU	LYS	conflict	UNP Q9K5F2
C	270	GLN	LYS	conflict	UNP Q9K5F2
C	289	GLU	ASP	conflict	UNP Q9K5F2
D	97	ASP	GLY	conflict	UNP Q9K5F2
D	236	GLU	LYS	conflict	UNP Q9K5F2
D	270	GLN	LYS	conflict	UNP Q9K5F2
D	289	GLU	ASP	conflict	UNP Q9K5F2
E	97	ASP	GLY	conflict	UNP Q9K5F2
E	236	GLU	LYS	conflict	UNP Q9K5F2
E	270	GLN	LYS	conflict	UNP Q9K5F2
E	289	GLU	ASP	conflict	UNP Q9K5F2
F	97	ASP	GLY	conflict	UNP Q9K5F2
F	236	GLU	LYS	conflict	UNP Q9K5F2
F	270	GLN	LYS	conflict	UNP Q9K5F2
F	289	GLU	ASP	conflict	UNP Q9K5F2
G	97	ASP	GLY	conflict	UNP Q9K5F2
G	236	GLU	LYS	conflict	UNP Q9K5F2
G	270	GLN	LYS	conflict	UNP Q9K5F2
G	289	GLU	ASP	conflict	UNP Q9K5F2
H	97	ASP	GLY	conflict	UNP Q9K5F2
H	236	GLU	LYS	conflict	UNP Q9K5F2
H	270	GLN	LYS	conflict	UNP Q9K5F2
H	289	GLU	ASP	conflict	UNP Q9K5F2
I	97	ASP	GLY	conflict	UNP Q9K5F2
I	236	GLU	LYS	conflict	UNP Q9K5F2
I	270	GLN	LYS	conflict	UNP Q9K5F2
I	289	GLU	ASP	conflict	UNP Q9K5F2
J	97	ASP	GLY	conflict	UNP Q9K5F2
J	236	GLU	LYS	conflict	UNP Q9K5F2
J	270	GLN	LYS	conflict	UNP Q9K5F2
J	289	GLU	ASP	conflict	UNP Q9K5F2
K	97	ASP	GLY	conflict	UNP Q9K5F2
K	236	GLU	LYS	conflict	UNP Q9K5F2
K	270	GLN	LYS	conflict	UNP Q9K5F2
K	289	GLU	ASP	conflict	UNP Q9K5F2
L	97	ASP	GLY	conflict	UNP Q9K5F2
L	236	GLU	LYS	conflict	UNP Q9K5F2
L	270	GLN	LYS	conflict	UNP Q9K5F2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	289	GLU	ASP	conflict	UNP Q9K5F2

- Molecule 2 is water.

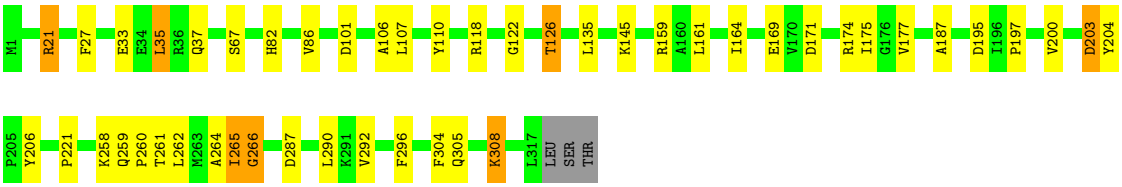
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	133	133	133	0	0
2	B	139	139	139	0	0
2	C	160	160	160	0	0
2	D	134	134	134	0	0
2	E	109	109	109	0	0
2	F	135	135	135	0	0
2	G	102	102	102	0	0
2	H	107	107	107	0	0
2	I	128	128	128	0	0
2	J	118	118	118	0	0
2	K	117	117	117	0	0
2	L	122	122	122	0	0

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 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.

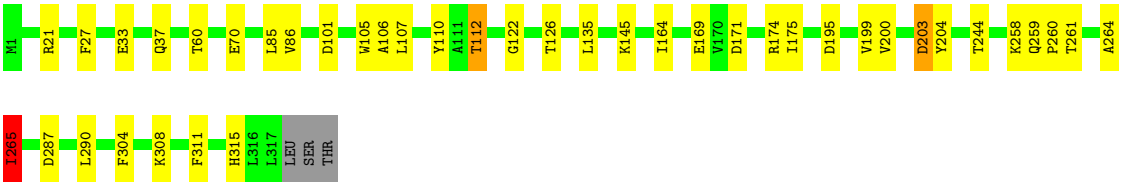
• Molecule 1: ACETYL XYLAN ESTERASE

Chain A:



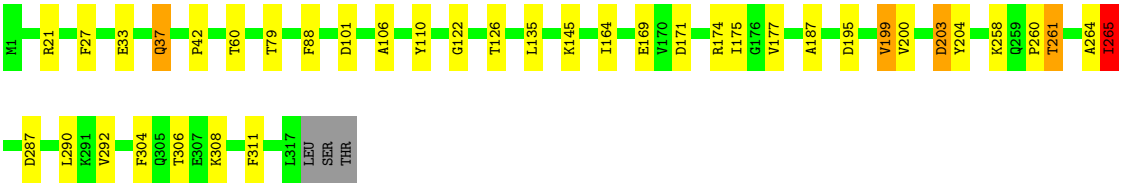
• Molecule 1: ACETYL XYLAN ESTERASE

Chain B:



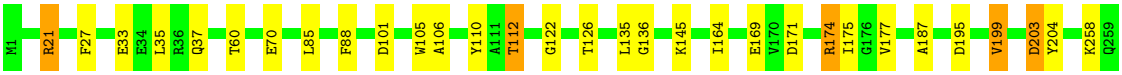
• Molecule 1: ACETYL XYLAN ESTERASE

Chain C:



• Molecule 1: ACETYL XYLAN ESTERASE

Chain D:

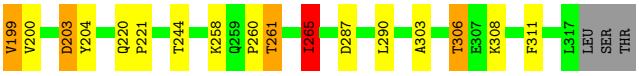


• Molecule 1: ACETYL XYLAN ESTERASE

Chain E:

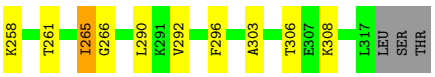
• Molecule 1: ACETYL XYLAN ESTERASE

Chain F:



• Molecule 1: ACETYL XYLAN ESTERASE

Chain G:

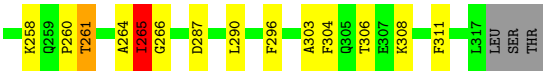


• Molecule 1: ACETYL XYLAN ESTERASE

Chain H:

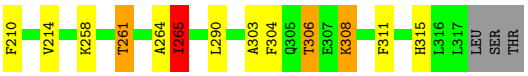
• Molecule 1: ACETYL XYLAN ESTERASE

Chain I:



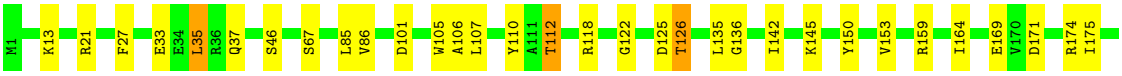
• Molecule 1: ACETYL XYLAN ESTERASE

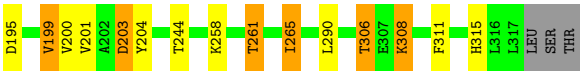
Chain J:



• Molecule 1: ACETYL XYLAN ESTERASE

Chain K:





• Molecule 1: ACETYL XYLAN ESTERASE

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	143.48Å 87.30Å 184.29Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.00-1.90) 92.2 (29.63-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.50 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.136 , 0.150 0.145 , 0.148	Depositor DCC
R_{free} test set	15354 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	14.5	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 13.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.540 for 1.000H, 1.000K, L 0.460 for -1.000H, -1.000K, 1.000H+L	Depositor
Outliers	0 of 304243 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31554	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.57	0/2584	0.63	1/3519 (0.0%)
1	B	0.55	1/2584 (0.0%)	0.63	1/3517 (0.0%)
1	C	0.50	1/2576 (0.0%)	0.60	1/3509 (0.0%)
1	D	0.53	1/2576 (0.0%)	0.62	2/3509 (0.1%)
1	E	0.54	5/2573 (0.2%)	0.64	3/3505 (0.1%)
1	F	0.58	4/2576 (0.2%)	0.63	1/3509 (0.0%)
1	G	0.51	0/2576	0.60	0/3509
1	H	0.49	1/2573 (0.0%)	0.60	0/3505
1	I	0.53	1/2573 (0.0%)	0.63	1/3505 (0.0%)
1	J	0.54	1/2573 (0.0%)	0.61	1/3505 (0.0%)
1	K	0.54	2/2573 (0.1%)	0.63	0/3505
1	L	0.54	2/2577 (0.1%)	0.63	1/3510 (0.0%)
All	All	0.54	19/30914 (0.1%)	0.62	12/42107 (0.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	230	ARG	CZ-NH2	-5.90	1.25	1.33
1	B	86	VAL	CB-CG1	-5.75	1.40	1.52
1	F	128	VAL	CB-CG1	-5.58	1.41	1.52
1	F	199	VAL	CB-CG1	-5.35	1.41	1.52
1	C	199	VAL	CB-CG1	-5.34	1.41	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	230	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	265	ILE	CB-CA-C	-5.51	100.57	111.60
1	E	230	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	174	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	265	ILE	CB-CA-C	-5.22	101.15	111.60

There are no chirality outliers.

There are no planarity outliers.

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	2512	0	2406	34	0
1	B	2512	0	2420	32	0
1	C	2504	0	2398	31	0
1	D	2504	0	2398	35	0
1	E	2501	0	2396	28	0
1	F	2504	0	2398	36	0
1	G	2504	0	2398	34	0
1	H	2501	0	2396	27	0
1	I	2501	0	2396	39	0
1	J	2501	0	2396	42	0
1	K	2501	0	2396	37	0
1	L	2505	0	2400	42	0
2	A	133	0	0	2	0
2	B	139	0	0	1	0
2	C	160	0	0	2	0
2	D	134	0	0	1	0
2	E	109	0	0	0	0
2	F	135	0	0	1	0
2	G	102	0	0	2	0
2	H	107	0	0	0	0
2	I	128	0	0	0	0
2	J	118	0	0	2	0
2	K	117	0	0	3	0
2	L	122	0	0	1	0
All	All	31554	0	28798	359	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 6.

The worst 5 of 359 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:G:135:LEU:CD2	1:J:135:LEU:CD2	2.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:CD2	1:E:135:LEU:CD2	2.40	0.99
1:I:135:LEU:CD2	1:L:135:LEU:CD2	2.40	0.98
1:A:135:LEU:CD2	1:D:135:LEU:CD2	2.43	0.97
1:G:244:THR:HG22	2:G:2060:HOH:O	1.70	0.92

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	315/320 (98%)	305 (97%)	9 (3%)	1 (0%)	41	31
1	B	315/320 (98%)	305 (97%)	9 (3%)	1 (0%)	41	31
1	C	315/320 (98%)	305 (97%)	9 (3%)	1 (0%)	41	31
1	D	315/320 (98%)	304 (96%)	10 (3%)	1 (0%)	41	31
1	E	315/320 (98%)	306 (97%)	8 (2%)	1 (0%)	41	31
1	F	315/320 (98%)	306 (97%)	8 (2%)	1 (0%)	41	31
1	G	315/320 (98%)	304 (96%)	10 (3%)	1 (0%)	41	31
1	H	315/320 (98%)	304 (96%)	10 (3%)	1 (0%)	41	31
1	I	315/320 (98%)	304 (96%)	10 (3%)	1 (0%)	41	31
1	J	315/320 (98%)	304 (96%)	10 (3%)	1 (0%)	41	31
1	K	315/320 (98%)	305 (97%)	9 (3%)	1 (0%)	41	31
1	L	315/320 (98%)	306 (97%)	8 (2%)	1 (0%)	41	31
All	All	3780/3840 (98%)	3658 (97%)	110 (3%)	12 (0%)	41	31

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	122	GLY

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Mol	Chain	Res	Type
1	B	122	GLY
1	E	122	GLY
1	G	122	GLY
1	H	122	GLY

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	260/270 (96%)	246 (95%)	14 (5%)	22	13
1	B	260/270 (96%)	248 (95%)	12 (5%)	27	17
1	C	258/270 (96%)	245 (95%)	13 (5%)	24	15
1	D	258/270 (96%)	244 (95%)	14 (5%)	22	13
1	E	257/270 (95%)	243 (95%)	14 (5%)	22	13
1	F	258/270 (96%)	244 (95%)	14 (5%)	22	13
1	G	258/270 (96%)	243 (94%)	15 (6%)	20	10
1	H	257/270 (95%)	243 (95%)	14 (5%)	22	13
1	I	257/270 (95%)	243 (95%)	14 (5%)	22	13
1	J	257/270 (95%)	243 (95%)	14 (5%)	22	13
1	K	257/270 (95%)	242 (94%)	15 (6%)	20	10
1	L	258/270 (96%)	243 (94%)	15 (6%)	20	10
All	All	3095/3240 (96%)	2927 (95%)	168 (5%)	22	13

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	112	THR
1	K	112	THR
1	I	203	ASP
1	J	126	THR
1	K	265	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	220	GLN
1	I	220	GLN
1	L	220	GLN
1	H	220	GLN
1	J	37	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	317/320 (99%)	-0.69	0	100	100	7, 12, 21, 34	0
1	B	317/320 (99%)	-0.69	0	100	100	7, 11, 19, 34	0
1	C	317/320 (99%)	-0.67	0	100	100	7, 11, 19, 31	0
1	D	317/320 (99%)	-0.70	0	100	100	7, 11, 19, 35	0
1	E	317/320 (99%)	-0.71	0	100	100	7, 12, 21, 27	0
1	F	317/320 (99%)	-0.68	0	100	100	8, 12, 21, 37	0
1	G	317/320 (99%)	-0.65	0	100	100	11, 16, 25, 35	0
1	H	317/320 (99%)	-0.69	0	100	100	9, 14, 24, 33	0
1	I	317/320 (99%)	-0.70	0	100	100	7, 12, 21, 36	0
1	J	317/320 (99%)	-0.70	0	100	100	8, 13, 22, 38	0
1	K	317/320 (99%)	-0.68	0	100	100	8, 13, 22, 35	0
1	L	317/320 (99%)	-0.70	0	100	100	7, 12, 21, 37	0
All	All	3804/3840 (99%)	-0.69	0	100	100	7, 12, 22, 38	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.