



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:43 PM UTC

PDB ID : 3LPM / pdb_00003lpm
Title : Crystal structure of putative methyltransferase small domain protein from *Listeria monocytogenes*
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-02-05
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

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

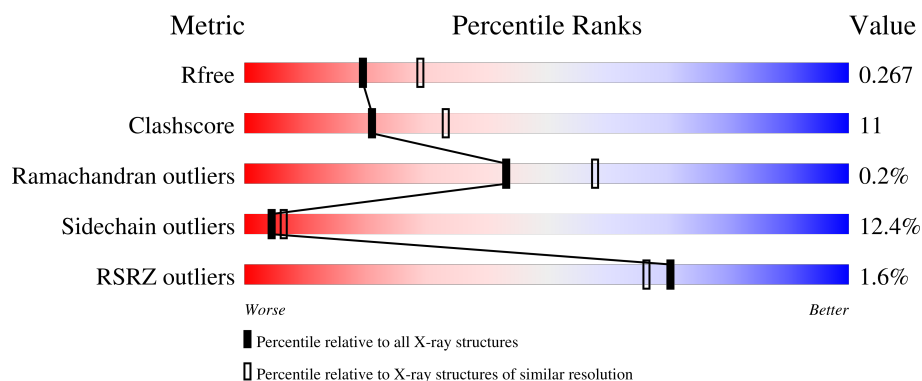
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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 ≥ 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	259	% 58% 22% 5% 14%
1	B	259	2% 59% 22% • • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3675 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 Putative methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	Se	0	0	0
			1770	1139	302	323	3	3			
1	B	222	Total	C	N	O	S	Se	0	1	0
			1777	1144	304	323	3	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP C1KXY4
A	2	SER	-	expression tag	UNP C1KXY4
A	7	LYS	GLU	conflict	UNP C1KXY4
A	253	GLY	-	expression tag	UNP C1KXY4
A	254	HIS	-	expression tag	UNP C1KXY4
A	255	HIS	-	expression tag	UNP C1KXY4
A	256	HIS	-	expression tag	UNP C1KXY4
A	257	HIS	-	expression tag	UNP C1KXY4
A	258	HIS	-	expression tag	UNP C1KXY4
A	259	HIS	-	expression tag	UNP C1KXY4
B	1	MSE	-	expression tag	UNP C1KXY4
B	2	SER	-	expression tag	UNP C1KXY4
B	7	LYS	GLU	conflict	UNP C1KXY4
B	253	GLY	-	expression tag	UNP C1KXY4
B	254	HIS	-	expression tag	UNP C1KXY4
B	255	HIS	-	expression tag	UNP C1KXY4
B	256	HIS	-	expression tag	UNP C1KXY4
B	257	HIS	-	expression tag	UNP C1KXY4
B	258	HIS	-	expression tag	UNP C1KXY4
B	259	HIS	-	expression tag	UNP C1KXY4

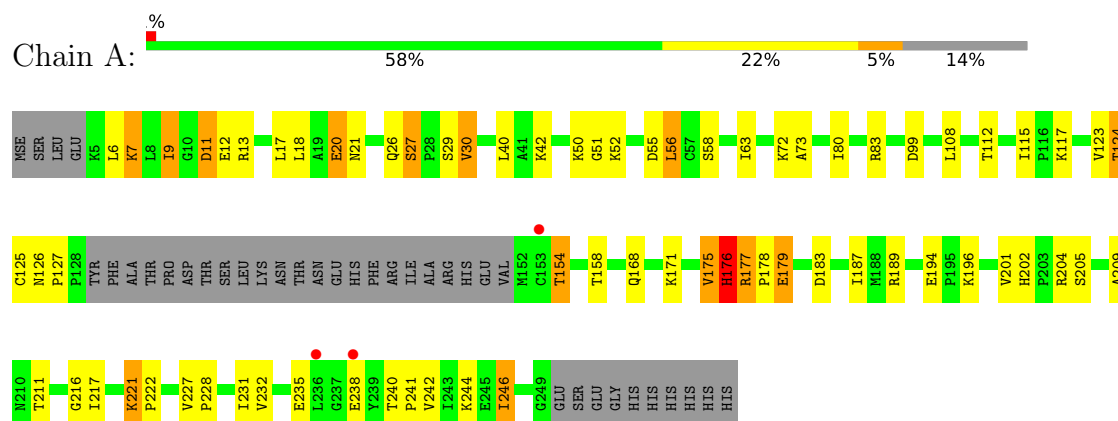
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total 65	O 65	0	0
2	B	63	Total 63	O 63	0	0

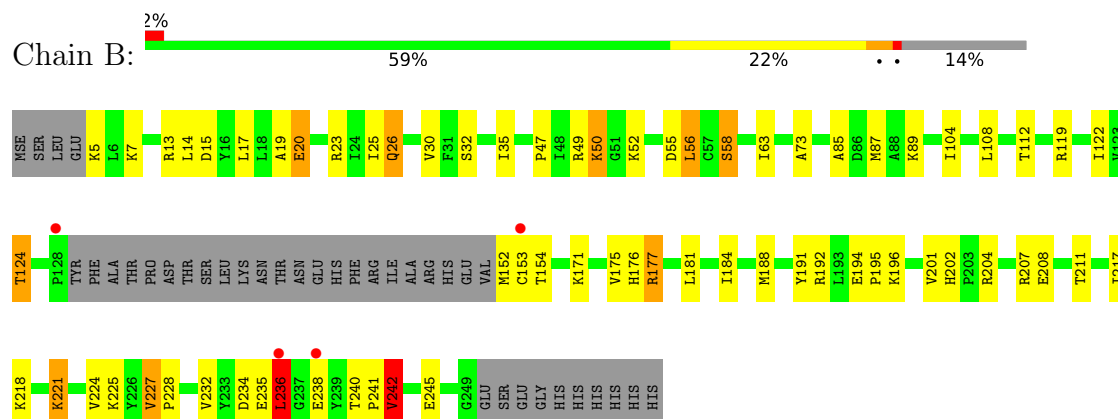
3 Residue-property plots

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: Putative methyltransferase



• Molecule 1: Putative methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.25Å 76.28Å 143.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 19.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.96-2.40) 98.0 (19.96-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.271 0.218 , 0.267	Depositor DCC
R_{free} test set	1543 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3675	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.01% 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

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	1.08	3/1795 (0.2%)	1.03	10/2420 (0.4%)
1	B	1.09	1/1806 (0.1%)	1.03	11/2435 (0.5%)
All	All	1.08	4/3601 (0.1%)	1.03	21/4855 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	PRO	CA-C	5.77	1.55	1.51
1	B	242	VAL	CA-CB	-5.35	1.47	1.54
1	A	126	ASN	C-O	-5.16	1.19	1.24
1	A	123	VAL	CA-CB	-5.00	1.48	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	VAL	N-CA-C	9.53	119.49	110.53
1	B	58	SER	N-CA-C	8.09	120.10	111.28
1	A	30	VAL	N-CA-C	7.53	118.82	111.67
1	B	56	LEU	N-CA-C	6.91	118.89	111.36
1	B	236	LEU	N-CA-C	-6.68	104.03	111.71
1	A	30	VAL	CB-CA-C	-6.40	104.25	111.80
1	A	176	HIS	N-CA-C	6.30	116.88	108.38
1	A	177	ARG	CA-C-N	6.28	126.76	119.47
1	A	177	ARG	C-N-CA	6.28	126.76	119.47
1	B	177	ARG	CA-C-N	5.82	125.95	119.32
1	B	177	ARG	C-N-CA	5.82	125.95	119.32
1	B	175	VAL	CB-CA-C	-5.57	103.26	110.84
1	A	125	CYS	N-CA-C	5.43	117.48	108.13
1	A	56	LEU	N-CA-C	5.41	117.25	111.36
1	A	238	GLU	N-CA-C	5.34	118.37	110.46
1	B	202	HIS	CA-C-N	5.26	124.71	119.24
1	B	202	HIS	C-N-CA	5.26	124.71	119.24
1	A	232	VAL	N-CA-C	5.20	115.47	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	VAL	CB-CA-C	-5.09	103.25	110.83
1	B	30	VAL	N-CA-C	5.04	115.33	110.74
1	B	181	LEU	N-CA-C	5.03	117.41	111.33

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	1770	0	1871	43	0
1	B	1777	0	1878	37	0
2	A	65	0	0	3	0
2	B	63	0	0	1	0
All	All	3675	0	3749	80	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 11.

All (80) 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:9:ILE:O	1:A:9:ILE:HG12	1.53	1.01
1:A:227:VAL:HG13	1:A:228:PRO:HD2	1.51	0.90
1:A:9:ILE:O	1:A:9:ILE:CG1	2.30	0.80
1:B:196:LYS:HG3	1:B:217:ILE:HG12	1.66	0.75
1:A:55:ASP:OD1	1:A:124:THR:HG22	1.86	0.75
1:A:40:LEU:HD22	1:A:175:VAL:HG23	1.70	0.73
1:B:55:ASP:OD1	1:B:124:THR:HG22	1.90	0.71
1:B:191:TYR:O	1:B:192:ARG:HB2	1.93	0.68
1:A:196:LYS:HG3	1:A:217:ILE:HD13	1.75	0.68
1:B:196:LYS:HG3	1:B:217:ILE:CG1	2.26	0.65
1:A:50:LYS:HG3	1:A:51:GLY:H	1.61	0.65
1:B:63:ILE:HG21	1:B:124:THR:HG21	1.79	0.64
1:A:11:ASP:OD2	1:A:29:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ALA:HB3	1:B:20:GLU:OE1	2.01	0.60
1:B:85:ALA:O	1:B:89:LYS:HG3	2.02	0.60
1:A:196:LYS:NZ	1:A:221:LYS:O	2.30	0.59
1:A:55:ASP:OD1	1:A:124:THR:CG2	2.51	0.58
1:A:11:ASP:OD1	1:A:11:ASP:C	2.45	0.57
1:B:47:PRO:HD3	1:B:122:ILE:HD12	1.87	0.57
1:A:227:VAL:HG13	1:A:228:PRO:CD	2.32	0.57
1:A:183:ASP:O	1:A:187:ILE:HG13	2.04	0.56
1:A:52:LYS:HE2	2:A:313:HOH:O	2.06	0.56
1:A:117:LYS:HG2	2:A:272:HOH:O	2.05	0.56
1:A:17:LEU:HB3	1:A:20:GLU:HG2	1.86	0.56
1:A:227:VAL:CG1	1:A:228:PRO:HD2	2.30	0.55
1:B:235:GLU:H	1:B:235:GLU:CD	2.15	0.55
1:A:240:THR:HG22	1:A:241:PRO:N	2.22	0.54
1:B:176[B]:HIS:CG	1:B:184:ILE:HD13	2.42	0.53
1:B:201:VAL:HB	1:B:211:THR:HB	1.89	0.53
1:A:50:LYS:CG	1:A:51:GLY:H	2.21	0.53
1:B:14:LEU:O	1:B:23:ARG:NH1	2.42	0.52
1:B:50:LYS:O	1:B:73:ALA:HB2	2.10	0.51
1:B:204:ARG:HB2	1:B:207:ARG:HD3	1.93	0.51
1:A:50:LYS:O	1:A:73:ALA:HB2	2.11	0.50
1:B:176[A]:HIS:CG	1:B:177:ARG:H	2.30	0.49
1:A:241:PRO:HA	1:A:244:LYS:HD3	1.94	0.49
1:B:20:GLU:CD	1:B:20:GLU:N	2.70	0.49
1:B:218:LYS:NZ	2:B:301:HOH:O	2.45	0.49
1:B:26:GLN:HA	1:B:87:MSE:HE1	1.95	0.48
1:A:99:ASP:HB2	2:A:262:HOH:O	2.12	0.47
1:A:112:THR:HA	1:A:115:ILE:O	2.15	0.46
1:A:27:SER:OG	1:A:30:VAL:HG23	2.15	0.46
1:A:55:ASP:HA	1:A:124:THR:HG22	1.98	0.46
1:B:55:ASP:OD1	1:B:124:THR:CG2	2.62	0.46
1:A:176:HIS:CG	1:A:177:ARG:H	2.33	0.46
1:A:11:ASP:OD1	1:A:11:ASP:O	2.32	0.46
1:A:154:THR:O	1:A:158:THR:HG23	2.16	0.46
1:A:242:VAL:O	1:A:246:ILE:HG12	2.15	0.46
1:B:224:VAL:HG12	1:B:225:LYS:N	2.30	0.46
1:B:56:LEU:HA	1:B:56:LEU:HD23	1.75	0.45
1:B:221:LYS:HD3	1:B:221:LYS:HA	1.41	0.45
1:A:221:LYS:HA	1:A:222:PRO:HD3	1.84	0.44
1:A:227:VAL:CG1	1:A:228:PRO:CD	2.94	0.44
1:B:15:ASP:O	1:B:23:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:THR:HG22	1:B:242:VAL:HG23	1.98	0.44
1:B:52:LYS:NZ	1:B:119:ARG:NH2	2.66	0.44
1:B:184:ILE:O	1:B:188:MSE:HG3	2.17	0.44
1:B:17:LEU:HB3	1:B:20:GLU:HG2	1.99	0.44
1:A:179:GLU:H	1:A:179:GLU:HG3	1.41	0.44
1:B:152:MSE:HB3	1:B:153:CYS:H	1.58	0.44
1:A:205:SER:HA	1:A:231:ILE:HD12	2.00	0.43
1:A:7:LYS:HA	1:A:7:LYS:HD2	1.82	0.43
1:B:234:ASP:C	1:B:234:ASP:OD1	2.61	0.43
1:B:240:THR:HG22	1:B:241:PRO:N	2.32	0.43
1:A:177:ARG:HA	1:A:178:PRO:HD3	1.85	0.43
1:A:202:HIS:CE1	1:A:209:ALA:HB2	2.54	0.43
1:A:196:LYS:HE3	1:A:196:LYS:HB3	1.74	0.42
1:B:171:LYS:HG3	1:B:217:ILE:HD13	2.00	0.42
1:A:221:LYS:HA	1:A:221:LYS:HD3	1.69	0.42
1:B:227:VAL:HG13	1:B:228:PRO:HD2	2.01	0.42
1:A:63:ILE:HG21	1:A:124:THR:HG21	2.02	0.42
1:A:201:VAL:HB	1:A:211:THR:HB	2.02	0.42
1:B:196:LYS:CG	1:B:217:ILE:HG12	2.45	0.42
1:A:194:GLU:O	1:A:216:GLY:HA2	2.20	0.42
1:B:25:ILE:O	1:B:87:MSE:HE2	2.20	0.42
1:A:50:LYS:HG3	1:A:51:GLY:N	2.32	0.41
1:B:194:GLU:HA	1:B:195:PRO:HD3	1.92	0.41
1:B:235:GLU:HG2	1:B:236:LEU:N	2.35	0.41
1:B:47:PRO:HD3	1:B:122:ILE:CD1	2.50	0.40
1:A:9:ILE:HD11	1:A:83:ARG:HH21	1.86	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	218/259 (84%)	213 (98%)	4 (2%)	1 (0%)	24	37
1	B	219/259 (85%)	214 (98%)	5 (2%)	0	100	100
All	All	437/518 (84%)	427 (98%)	9 (2%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLU

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	198/228 (87%)	171 (86%)	27 (14%)	3	5
1	B	199/228 (87%)	177 (89%)	22 (11%)	6	9
All	All	397/456 (87%)	348 (88%)	49 (12%)	4	6

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	LYS
1	A	9	ILE
1	A	11	ASP
1	A	13	ARG
1	A	18	LEU
1	A	20	GLU
1	A	21	ASN
1	A	26	GLN
1	A	27	SER
1	A	42	LYS
1	A	56	LEU
1	A	58	SER
1	A	72	LYS
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	124	THR
1	A	154	THR
1	A	168	GLN
1	A	171	LYS
1	A	176	HIS
1	A	179	GLU
1	A	189	ARG
1	A	204	ARG
1	A	221	LYS
1	A	235	GLU
1	A	246	ILE
1	B	5	LYS
1	B	7	LYS
1	B	13	ARG
1	B	20	GLU
1	B	26	GLN
1	B	32	SER
1	B	35	ILE
1	B	49	ARG
1	B	50	LYS
1	B	58	SER
1	B	104	ILE
1	B	108	LEU
1	B	112	THR
1	B	124	THR
1	B	154	THR
1	B	208	GLU
1	B	221	LYS
1	B	227	VAL
1	B	236	LEU
1	B	238	GLU
1	B	242	VAL
1	B	245	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	B	21	ASN
1	B	173	ASN

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](#)

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	219/259 (84%)	-0.17	3 (1%) 73 69	26, 38, 62, 86	0
1	B	219/259 (84%)	-0.18	4 (1%) 67 63	22, 37, 64, 87	1 (0%)
All	All	438/518 (84%)	-0.17	7 (1%) 70 66	22, 37, 64, 87	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	CYS	3.2
1	B	238	GLU	3.2
1	B	128	PRO	3.1
1	B	236	LEU	3.1
1	A	236	LEU	2.8
1	A	153	CYS	2.6
1	A	238	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.