Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:38 am BST

PDB ID	:	5NEN
Title	:	Crystal structure of the soluble domain of LipC, a membrane fusion protein of a type I secretion system
Authors	:	Murata, D.; Akutsu, M.; Takano, K.
Deposited on	:	2017-03-11
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

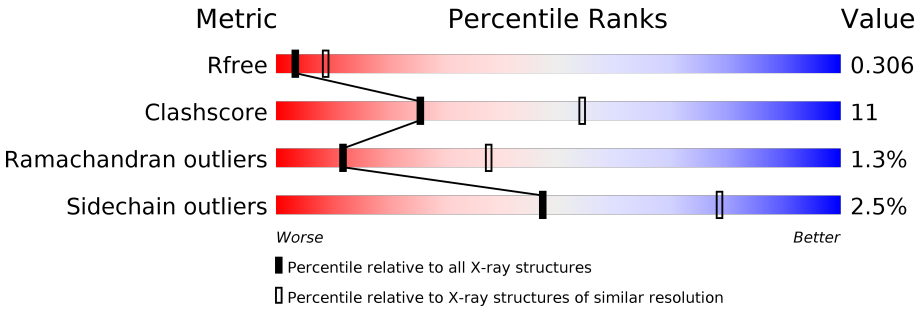
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	448	46% 13% • 41%
1	B	448	38% 9% • 52%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3604 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 Lipase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			1982	1220	360	396	6			
1	B	213	Total	C	N	O	S	0	0	0
			1622	1000	292	325	5			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP Q54457
A	?	-	GLY	deletion	UNP Q54457
A	?	-	TRP	deletion	UNP Q54457
A	?	-	LEU	deletion	UNP Q54457
A	?	-	VAL	deletion	UNP Q54457
A	?	-	VAL	deletion	UNP Q54457
A	?	-	GLY	deletion	UNP Q54457
A	?	-	ILE	deletion	UNP Q54457
A	?	-	GLY	deletion	UNP Q54457
A	?	-	LEU	deletion	UNP Q54457
A	?	-	PHE	deletion	UNP Q54457
A	?	-	GLY	deletion	UNP Q54457
A	?	-	PHE	deletion	UNP Q54457
A	?	-	LEU	deletion	UNP Q54457
A	?	-	ALA	deletion	UNP Q54457
A	?	-	TRP	deletion	UNP Q54457
A	?	-	ALA	deletion	UNP Q54457
A	?	-	ALA	deletion	UNP Q54457
A	?	-	PHE	deletion	UNP Q54457
A	?	-	ALA	deletion	UNP Q54457
A	?	-	PRO	deletion	UNP Q54457
A	423	LEU	-	expression tag	UNP Q54457
A	424	GLU	-	expression tag	UNP Q54457
A	425	ILE	-	expression tag	UNP Q54457
A	426	LYS	-	expression tag	UNP Q54457

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Chain	Residue	Modelled	Actual	Comment	Reference
A	427	ARG	-	expression tag	UNP Q54457
A	428	ALA	-	expression tag	UNP Q54457
A	429	SER	-	expression tag	UNP Q54457
A	430	GLN	-	expression tag	UNP Q54457
A	431	PRO	-	expression tag	UNP Q54457
A	432	GLU	-	expression tag	UNP Q54457
A	433	LEU	-	expression tag	UNP Q54457
A	434	ALA	-	expression tag	UNP Q54457
A	435	PRO	-	expression tag	UNP Q54457
A	436	GLU	-	expression tag	UNP Q54457
A	437	ASP	-	expression tag	UNP Q54457
A	438	PRO	-	expression tag	UNP Q54457
A	439	GLU	-	expression tag	UNP Q54457
A	440	ASP	-	expression tag	UNP Q54457
A	441	VAL	-	expression tag	UNP Q54457
A	442	GLU	-	expression tag	UNP Q54457
A	443	HIS	-	expression tag	UNP Q54457
A	444	HIS	-	expression tag	UNP Q54457
A	445	HIS	-	expression tag	UNP Q54457
A	446	HIS	-	expression tag	UNP Q54457
A	447	HIS	-	expression tag	UNP Q54457
A	448	HIS	-	expression tag	UNP Q54457
B	?	-	MET	deletion	UNP Q54457
B	?	-	GLY	deletion	UNP Q54457
B	?	-	TRP	deletion	UNP Q54457
B	?	-	LEU	deletion	UNP Q54457
B	?	-	VAL	deletion	UNP Q54457
B	?	-	VAL	deletion	UNP Q54457
B	?	-	GLY	deletion	UNP Q54457
B	?	-	ILE	deletion	UNP Q54457
B	?	-	GLY	deletion	UNP Q54457
B	?	-	LEU	deletion	UNP Q54457
B	?	-	PHE	deletion	UNP Q54457
B	?	-	GLY	deletion	UNP Q54457
B	?	-	PHE	deletion	UNP Q54457
B	?	-	LEU	deletion	UNP Q54457
B	?	-	ALA	deletion	UNP Q54457
B	?	-	TRP	deletion	UNP Q54457
B	?	-	ALA	deletion	UNP Q54457
B	?	-	ALA	deletion	UNP Q54457
B	?	-	PHE	deletion	UNP Q54457
B	?	-	ALA	deletion	UNP Q54457

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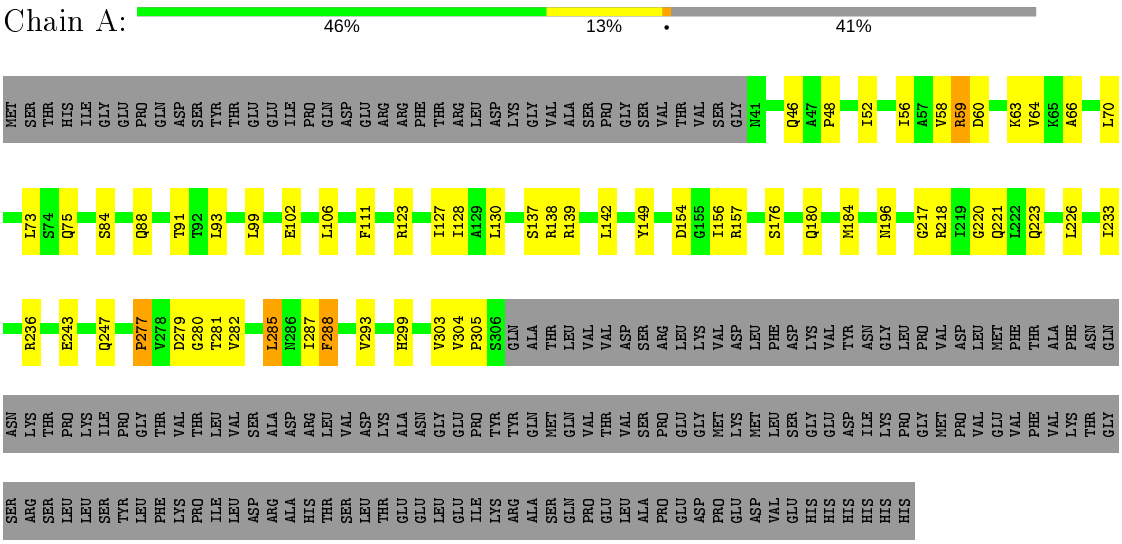
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP Q54457
B	423	LEU	-	expression tag	UNP Q54457
B	424	GLU	-	expression tag	UNP Q54457
B	425	ILE	-	expression tag	UNP Q54457
B	426	LYS	-	expression tag	UNP Q54457
B	427	ARG	-	expression tag	UNP Q54457
B	428	ALA	-	expression tag	UNP Q54457
B	429	SER	-	expression tag	UNP Q54457
B	430	GLN	-	expression tag	UNP Q54457
B	431	PRO	-	expression tag	UNP Q54457
B	432	GLU	-	expression tag	UNP Q54457
B	433	LEU	-	expression tag	UNP Q54457
B	434	ALA	-	expression tag	UNP Q54457
B	435	PRO	-	expression tag	UNP Q54457
B	436	GLU	-	expression tag	UNP Q54457
B	437	ASP	-	expression tag	UNP Q54457
B	438	PRO	-	expression tag	UNP Q54457
B	439	GLU	-	expression tag	UNP Q54457
B	440	ASP	-	expression tag	UNP Q54457
B	441	VAL	-	expression tag	UNP Q54457
B	442	GLU	-	expression tag	UNP Q54457
B	443	HIS	-	expression tag	UNP Q54457
B	444	HIS	-	expression tag	UNP Q54457
B	445	HIS	-	expression tag	UNP Q54457
B	446	HIS	-	expression tag	UNP Q54457
B	447	HIS	-	expression tag	UNP Q54457
B	448	HIS	-	expression tag	UNP Q54457

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

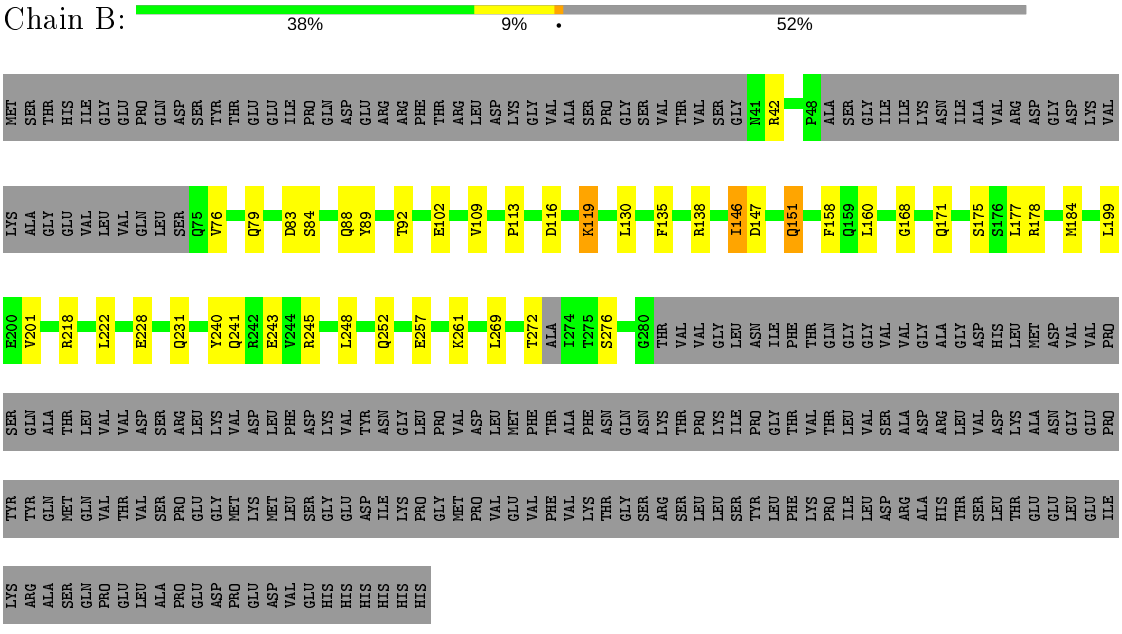
- Molecule 1: Lipase C

Chain A:



- Molecule 1: Lipase C

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	126.31Å 126.31Å 71.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.35 – 2.90 41.35 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.35-2.90) 100.0 (41.35-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.252 , 0.301 0.257 , 0.306	Depositor DCC
R_{free} test set	1382 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	82.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.080 for -h,-k,l 0.345 for h,-h-k,-l 0.087 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3604	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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

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	0.53	0/1998	0.72	0/2706
1	B	0.53	0/1635	0.74	0/2202
All	All	0.53	0/3633	0.73	0/4908

There are no bond length outliers.

There are no bond angle outliers.

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	1982	0	1914	46	0
1	B	1622	0	1537	34	0
All	All	3604	0	3451	75	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 (75) 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:73:LEU:HD23	1:A:75:GLN:H	1.34	0.92
1:A:88:GLN:OE1	1:B:218:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:HA	1:B:116:ASP:HB3	1.68	0.76
1:A:102:GLU:OE1	1:A:138:ARG:NH1	2.22	0.72
1:A:154:ASP:OD1	1:A:157:ARG:NH1	2.27	0.68
1:A:63:LYS:HA	1:A:281:THR:HA	1.77	0.67
1:B:241:GLN:OE1	1:B:245:ARG:NH1	2.27	0.65
1:A:282:VAL:HG12	1:A:303:VAL:HG12	1.79	0.64
1:A:277:PRO:HD2	1:A:303:VAL:HG21	1.81	0.63
1:B:147:ASP:O	1:B:151:GLN:HG2	1.99	0.62
1:A:59:ARG:HA	1:A:285:LEU:HD21	1.83	0.60
1:A:64:VAL:HB	1:A:280:GLY:H	1.68	0.59
1:B:102:GLU:HB3	1:B:240:TYR:OH	2.04	0.57
1:A:52:ILE:HG12	1:A:293:VAL:HG12	1.86	0.56
1:B:138:ARG:NH2	1:B:243:GLU:OE2	2.38	0.56
1:A:60:ASP:H	1:A:285:LEU:HD11	1.69	0.56
1:A:137:SER:OG	1:B:151:GLN:NE2	2.38	0.56
1:B:228:GLU:O	1:B:231:GLN:HG2	2.07	0.55
1:A:123:ARG:NH2	1:B:158:PHE:O	2.31	0.53
1:A:156:ILE:HG21	1:A:226:LEU:HG	1.89	0.53
1:A:64:VAL:HB	1:A:280:GLY:O	2.08	0.53
1:B:84:SER:O	1:B:88:GLN:HG3	2.09	0.53
1:A:56:ILE:HG22	1:A:58:VAL:H	1.74	0.53
1:A:243:GLU:O	1:A:247:GLN:HG3	2.09	0.52
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.74	0.52
1:A:84:SER:O	1:A:88:GLN:HG3	2.09	0.52
1:A:102:GLU:CD	1:A:138:ARG:HH11	2.13	0.52
1:A:130:LEU:HD21	1:B:151:GLN:O	2.10	0.51
1:B:116:ASP:O	1:B:119:LYS:HD3	2.11	0.50
1:B:184:MET:CE	1:B:201:VAL:HG21	2.41	0.50
1:A:176:SER:O	1:A:180:GLN:HG2	2.12	0.50
1:A:220:GLY:HA2	1:A:223:GLN:OE1	2.11	0.50
1:A:106:LEU:O	1:A:139:ARG:NH2	2.45	0.49
1:A:46:GLN:HA	1:A:299:HIS:HA	1.94	0.49
1:B:109:VAL:HG23	1:B:135:PHE:CD2	2.48	0.48
1:B:151:GLN:H	1:B:151:GLN:HG2	1.40	0.48
1:B:79:GLN:NE2	1:B:83:ASP:OD1	2.44	0.48
1:B:184:MET:HE3	1:B:201:VAL:HG21	1.94	0.48
1:B:175:SER:O	1:B:178:ARG:HB3	2.14	0.47
1:A:218:ARG:HH22	1:B:261:LYS:HZ1	1.62	0.47
1:B:248:LEU:O	1:B:252:GLN:HG3	2.15	0.47
1:A:73:LEU:O	1:A:75:GLN:HG3	2.14	0.47
1:B:89:TYR:O	1:B:92:THR:OG1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HA	1:B:130:LEU:HD12	1.76	0.46
1:B:228:GLU:HA	1:B:231:GLN:HG2	1.98	0.46
1:B:269:LEU:O	1:B:272:THR:HG23	2.15	0.46
1:B:113:PRO:HA	1:B:116:ASP:CB	2.44	0.46
1:B:102:GLU:OE2	1:B:138:ARG:NH1	2.42	0.45
1:A:243:GLU:CG	1:A:247:GLN:HE21	2.29	0.45
1:A:64:VAL:N	1:A:280:GLY:O	2.50	0.45
1:A:196:ASN:C	1:A:196:ASN:OD1	2.54	0.45
1:A:217:GLY:O	1:A:221:GLN:HG2	2.17	0.45
1:A:243:GLU:HG2	1:A:247:GLN:HE21	1.82	0.45
1:A:111:PHE:CE2	1:A:128:ILE:HG23	2.52	0.44
1:A:99:LEU:HA	1:A:99:LEU:HD23	1.69	0.44
1:B:160:LEU:HD21	1:B:222:LEU:HB2	1.99	0.44
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.79	0.44
1:B:116:ASP:OD1	1:B:119:LYS:HE3	2.18	0.43
1:A:64:VAL:HG12	1:A:279:ASP:HA	2.01	0.42
1:A:91:THR:HG23	1:A:127:ILE:HG12	2.01	0.42
1:A:149:TYR:HB3	1:A:233:ILE:HD11	2.00	0.42
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.74	0.42
1:B:199:LEU:H	1:B:199:LEU:HD12	1.84	0.42
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.78	0.42
1:A:184:MET:HE2	1:A:184:MET:HB3	1.86	0.42
1:A:142:LEU:HD13	1:A:236:ARG:HH12	1.85	0.42
1:A:58:VAL:HG21	1:A:70:LEU:HD22	2.02	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.83	0.41
1:A:288:PHE:N	1:A:288:PHE:CD1	2.86	0.41
1:A:127:ILE:HD12	1:A:127:ILE:HA	1.83	0.41
1:A:58:VAL:HG23	1:A:70:LEU:HA	2.02	0.40
1:B:146:ILE:HG13	1:B:147:ASP:N	2.36	0.40
1:B:168:GLY:O	1:B:171:GLN:HB2	2.21	0.40
1:A:58:VAL:HG12	1:A:282:VAL:HG21	2.02	0.40
1:A:287:ILE:HG23	1:A:288:PHE:CD1	2.57	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	264/448 (59%)	248 (94%)	12 (4%)	4 (2%)	10 34
1	B	207/448 (46%)	202 (98%)	3 (1%)	2 (1%)	15 45
All	All	471/896 (53%)	450 (96%)	15 (3%)	6 (1%)	12 37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	PRO
1	A	66	ALA
1	B	276	SER
1	A	48	PRO
1	A	277	PRO
1	B	42	ARG

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	202/388 (52%)	198 (98%)	4 (2%)	55 82
1	B	163/388 (42%)	158 (97%)	5 (3%)	40 74
All	All	365/776 (47%)	356 (98%)	9 (2%)	47 78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	285	LEU
1	A	288	PHE
1	A	304	VAL
1	B	76	VAL
1	B	119	LYS

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Mol	Chain	Res	Type
1	B	146	ILE
1	B	151	GLN
1	B	257	GLU

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

Mol	Chain	Res	Type
1	A	230	GLN
1	A	247	GLN
1	B	151	GLN

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 carbohydrates 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.