



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 12:35 AM EDT

PDB ID : 2GML  
Title : Crystal Structure of Catalytic Domain of E.coli RluF  
Authors : Sunita, S.; Zhenxing, H.; Swaathi, J.; Cygler, M.; Matte, A.; Sivaraman, J.  
Deposited on : 2006-04-06  
Resolution : 2.60 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

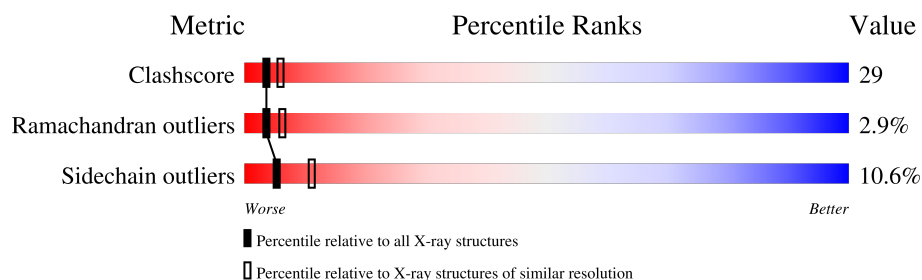
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	237	
1	B	237	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2750 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 Ribosomal large subunit pseudouridine synthase F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	Se	0	0	0
			1314	841	228	240	2	3			
1	B	175	Total	C	N	O	S	Se	0	0	0
			1311	839	228	239	2	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P32684
A	-10	GLY	-	expression tag	UNP P32684
A	-9	SER	-	expression tag	UNP P32684
A	-8	SER	-	expression tag	UNP P32684
A	-7	HIS	-	expression tag	UNP P32684
A	-6	HIS	-	expression tag	UNP P32684
A	-5	HIS	-	expression tag	UNP P32684
A	-4	HIS	-	expression tag	UNP P32684
A	-3	HIS	-	expression tag	UNP P32684
A	-2	HIS	-	expression tag	UNP P32684
A	-1	GLY	-	expression tag	UNP P32684
A	0	SER	-	expression tag	UNP P32684
A	88	MSE	MET	modified residue	UNP P32684
A	127	MSE	MET	modified residue	UNP P32684
A	144	MSE	MET	modified residue	UNP P32684
A	198	MSE	MET	modified residue	UNP P32684
B	-11	MET	-	expression tag	UNP P32684
B	-10	GLY	-	expression tag	UNP P32684
B	-9	SER	-	expression tag	UNP P32684
B	-8	SER	-	expression tag	UNP P32684
B	-7	HIS	-	expression tag	UNP P32684
B	-6	HIS	-	expression tag	UNP P32684
B	-5	HIS	-	expression tag	UNP P32684
B	-4	HIS	-	expression tag	UNP P32684
B	-3	HIS	-	expression tag	UNP P32684

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP P32684
B	-1	GLY	-	expression tag	UNP P32684
B	0	SER	-	expression tag	UNP P32684
B	88	MSE	MET	modified residue	UNP P32684
B	127	MSE	MET	modified residue	UNP P32684
B	144	MSE	MET	modified residue	UNP P32684
B	198	MSE	MET	modified residue	UNP P32684

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	67	Total O 67 67	0	0
2	B	58	Total O 58 58	0	0



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.71Å 65.71Å 215.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (45.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 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	0.49	0/1332	0.76	1/1800 (0.1%)
1	B	0.43	0/1329	0.73	0/1795
All	All	0.46	0/2661	0.75	1/3595 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	LEU	N-CA-C	-5.58	95.92	111.00

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	1314	0	1300	52	0
1	B	1311	0	1294	103	0
2	A	67	0	0	12	0
2	B	58	0	0	6	0
All	All	2750	0	2594	149	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 29.

All (149) 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:91:GLY:H	1:B:101:LYS:NZ	1.40	1.19
1:B:91:GLY:H	1:B:101:LYS:HZ3	1.03	0.94
1:A:9:LYS:HG3	1:A:13:ILE:HD11	1.54	0.87
1:A:121:ASN:HB2	2:A:275:HOH:O	1.77	0.84
1:B:91:GLY:N	1:B:101:LYS:NZ	2.24	0.84
1:B:9:LYS:HE2	1:B:13:ILE:O	1.78	0.81
1:A:119:GLY:O	1:A:120:LEU:HD23	1.81	0.81
1:A:99:THR:HB	2:A:227:HOH:O	1.81	0.81
1:B:91:GLY:H	1:B:101:LYS:HZ1	1.25	0.80
1:A:122:ARG:HG2	1:B:96:GLY:HA3	1.66	0.76
1:A:25:ILE:O	1:A:29:VAL:HG12	1.86	0.76
1:B:25:ILE:HG21	1:B:37:PRO:HG3	1.69	0.75
1:B:91:GLY:N	1:B:101:LYS:HZ3	1.82	0.74
1:A:29:VAL:HA	2:A:226:HOH:O	1.91	0.69
1:A:122:ARG:CG	1:B:96:GLY:HA3	2.22	0.69
1:B:92:VAL:HG23	1:B:94:ILE:HG23	1.75	0.68
1:A:9:LYS:HE2	1:A:13:ILE:O	1.94	0.68
1:A:2:LEU:HB3	2:A:258:HOH:O	1.95	0.67
1:B:94:ILE:HG21	1:B:127:MSE:HG2	1.78	0.66
1:A:88:MSE:HE1	1:A:128:CYS:SG	2.35	0.65
1:A:151:ILE:HD11	1:A:157:ARG:NH1	2.12	0.65
1:A:9:LYS:HG3	1:A:13:ILE:CD1	2.27	0.64
1:B:130:HIS:HA	2:B:279:HOH:O	1.98	0.64
1:B:17:THR:OG1	1:B:26:VAL:HG21	1.97	0.64
1:B:7:LEU:HD23	1:B:25:ILE:HD11	1.79	0.64
1:B:90:ALA:O	1:B:92:VAL:HG13	1.97	0.63
1:B:57:LEU:HD22	1:B:61:ILE:CD1	2.29	0.62
1:B:3:VAL:O	1:B:52:THR:HA	2.02	0.60
1:B:57:LEU:HD22	1:B:61:ILE:HD12	1.81	0.60
1:A:75:THR:HB	1:A:137:LYS:HB3	1.84	0.60
1:A:10:PRO:HD2	1:A:13:ILE:HD13	1.83	0.59
1:B:29:VAL:HG22	1:B:29:VAL:O	2.01	0.59
1:B:16:THR:O	1:B:24:ASN:HB2	2.03	0.59
1:B:91:GLY:N	1:B:101:LYS:HZ1	1.94	0.59
1:B:94:ILE:O	1:B:97:THR:HG22	2.03	0.58
1:B:35:VAL:CG1	1:B:51:LEU:HB3	2.34	0.58
1:B:41:LEU:HD22	1:B:45:SER:HB3	1.84	0.57
1:B:161:ASP:O	1:B:165:ILE:HG13	2.04	0.57
1:B:92:VAL:O	1:B:98:VAL:HA	2.05	0.57
1:B:165:ILE:O	1:B:169:LYS:HG3	2.05	0.56
1:B:95:LEU:HD12	1:B:120:LEU:HD13	1.87	0.56
1:B:97:THR:HG21	1:B:120:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HB2	1:B:120:LEU:HD13	1.89	0.55
1:A:3:VAL:O	1:A:52:THR:HA	2.06	0.55
1:B:2:LEU:HD23	1:B:54:HIS:CD2	2.41	0.55
1:B:25:ILE:O	1:B:29:VAL:HG12	2.07	0.55
1:B:35:VAL:HG12	1:B:36:PHE:N	2.21	0.55
1:B:17:THR:HG22	1:B:17:THR:O	2.07	0.55
1:B:125:ARG:O	1:B:129:GLU:HG3	2.08	0.54
1:B:6:ALA:HB1	1:B:48:LEU:HD21	1.90	0.54
1:A:72:TYR:HD2	1:A:138:LEU:HD22	1.72	0.54
1:A:10:PRO:HD2	1:A:13:ILE:CD1	2.38	0.53
1:A:66:ASN:HA	2:A:237:HOH:O	2.08	0.53
1:A:29:VAL:HG22	1:A:29:VAL:O	2.08	0.53
1:A:35:VAL:CG1	1:A:51:LEU:HB3	2.38	0.53
1:B:114:ILE:HG21	1:B:124:ILE:HD13	1.89	0.53
1:A:121:ASN:HB3	1:B:96:GLY:HA2	1.90	0.52
1:B:97:THR:HB	2:B:228:HOH:O	2.07	0.52
1:A:4:LEU:CD1	1:A:52:THR:HB	2.39	0.52
1:A:126:ARG:NH2	1:B:96:GLY:O	2.42	0.52
1:A:2:LEU:HD23	1:A:54:HIS:CD2	2.45	0.52
1:B:84:PHE:CZ	1:B:88:MSE:HE2	2.45	0.51
1:A:100:LYS:HE3	2:A:278:HOH:O	2.10	0.51
1:B:71:GLU:HB2	1:B:142:ARG:NH1	2.24	0.51
1:A:29:VAL:CA	2:A:226:HOH:O	2.55	0.51
1:B:25:ILE:CG2	1:B:37:PRO:HG3	2.38	0.51
1:B:116:LEU:HD12	1:B:116:LEU:H	1.76	0.51
1:B:121:ASN:C	1:B:123:GLN:H	2.15	0.51
1:B:80:ILE:HG21	1:B:106:LYS:HG3	1.93	0.51
1:B:20:GLY:HA3	2:B:254:HOH:O	2.10	0.50
1:B:95:LEU:CD1	1:B:120:LEU:HD13	2.41	0.50
1:A:95:LEU:HD12	1:A:120:LEU:HD13	1.93	0.50
1:B:25:ILE:HG23	1:B:26:VAL:N	2.27	0.50
1:B:4:LEU:HD13	1:B:52:THR:HB	1.94	0.50
1:B:48:LEU:HD13	1:B:143:ILE:HD12	1.94	0.50
1:B:34:ARG:HH11	1:B:34:ARG:HG3	1.78	0.49
1:B:121:ASN:C	1:B:123:GLN:N	2.65	0.49
1:A:35:VAL:HG13	1:A:51:LEU:HB3	1.95	0.49
1:A:4:LEU:HD12	1:A:52:THR:HB	1.95	0.49
1:A:100:LYS:HG3	2:A:254:HOH:O	2.12	0.49
1:B:14:VAL:CG1	1:B:43:LYS:HB2	2.43	0.48
1:A:9:LYS:CG	1:A:13:ILE:HD11	2.33	0.48
1:A:72:TYR:CD2	1:A:138:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HD12	1:B:25:ILE:HA	1.95	0.48
1:A:99:THR:HG22	1:A:100:LYS:O	2.13	0.48
1:B:17:THR:N	2:B:227:HOH:O	2.47	0.48
2:A:231:HOH:O	1:B:98:VAL:HG11	2.13	0.48
1:A:6:ALA:HB1	1:A:48:LEU:HD21	1.96	0.48
1:B:24:ASN:ND2	1:B:26:VAL:HB	2.28	0.48
1:B:77:ASP:OD1	1:B:78:LYS:N	2.46	0.48
1:B:64:ALA:O	1:B:68:HIS:HD2	1.97	0.47
1:B:71:GLU:OE2	1:B:113:ARG:HD3	2.14	0.47
1:B:71:GLU:OE1	1:B:142:ARG:NH1	2.47	0.47
1:A:65:GLY:HA2	2:A:249:HOH:O	2.14	0.47
1:B:20:GLY:O	1:B:22:ARG:N	2.47	0.47
1:B:94:ILE:O	1:B:94:ILE:HG13	2.14	0.47
1:B:35:VAL:HG11	1:B:51:LEU:HB3	1.96	0.47
1:B:108:ALA:HB1	1:B:109:PRO:HD2	1.97	0.47
1:A:92:VAL:HG22	1:A:94:ILE:HG23	1.97	0.47
1:B:55:GLY:O	1:B:58:VAL:HB	2.15	0.46
1:A:99:THR:HG22	1:A:100:LYS:N	2.29	0.46
1:B:29:VAL:O	1:B:29:VAL:CG2	2.63	0.46
1:B:68:HIS:CE1	1:B:170:LEU:HD22	2.51	0.46
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.16	0.46
1:A:24:ASN:OD1	1:A:27:ASP:OD1	2.34	0.45
1:B:84:PHE:O	1:B:88:MSE:HB2	2.16	0.45
1:B:25:ILE:HG21	1:B:37:PRO:CG	2.44	0.45
1:B:11:VAL:HG23	2:B:239:HOH:O	2.16	0.45
1:B:109:PRO:HB2	1:B:110:PHE:HD1	1.81	0.45
1:A:80:ILE:HD13	1:A:112:PHE:HB3	1.98	0.45
1:B:35:VAL:CG1	1:B:36:PHE:N	2.79	0.45
1:B:92:VAL:HG23	1:B:94:ILE:CG2	2.46	0.45
1:B:97:THR:CG2	1:B:120:LEU:HD11	2.47	0.45
1:B:102:CYS:HB3	1:B:116:LEU:HB3	1.98	0.45
1:A:24:ASN:ND2	1:A:27:ASP:OD1	2.50	0.44
1:B:88:MSE:HB3	1:B:104:VAL:HG21	1.98	0.44
1:B:74:VAL:HB	1:B:112:PHE:CE2	2.53	0.44
1:B:4:LEU:CD1	1:B:52:THR:HB	2.48	0.44
1:B:29:VAL:O	1:B:30:ASN:C	2.57	0.43
1:B:110:PHE:N	1:B:110:PHE:CD1	2.86	0.43
1:B:44:ASP:OD2	1:B:125:ARG:CZ	2.65	0.43
1:B:97:THR:CB	2:B:228:HOH:O	2.65	0.43
1:B:41:LEU:CD2	1:B:45:SER:HB3	2.48	0.43
1:A:74:VAL:HG22	1:A:138:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:O	1:B:152:PRO:HD3	2.19	0.43
1:B:69:GLU:OE1	1:B:142:ARG:NH2	2.52	0.43
1:B:9:LYS:HA	1:B:10:PRO:HD3	1.75	0.42
1:B:94:ILE:O	1:B:95:LEU:C	2.57	0.42
1:A:92:VAL:HA	1:A:93:PRO:HD3	1.77	0.42
1:B:2:LEU:HD21	1:B:57:LEU:HD12	2.00	0.42
1:A:121:ASN:HB3	1:B:96:GLY:CA	2.49	0.42
1:B:130:HIS:HD2	1:B:131:PHE:CE1	2.38	0.41
1:A:48:LEU:HD11	1:A:146:VAL:HG12	2.03	0.41
1:A:9:LYS:HA	1:A:10:PRO:HD3	1.96	0.41
1:B:77:ASP:OD2	1:B:134:GLU:CB	2.69	0.41
1:B:14:VAL:HG13	1:B:43:LYS:HB2	2.03	0.41
1:B:80:ILE:HB	1:B:106:LYS:HE3	2.03	0.41
1:B:101:LYS:HA	1:B:101:LYS:HD3	1.74	0.41
1:B:120:LEU:HD12	1:B:123:GLN:HG3	2.03	0.41
1:A:71:GLU:HB3	1:A:142:ARG:HB3	2.03	0.41
1:B:29:VAL:HG23	1:B:156:TRP:CD1	2.56	0.41
1:A:150:GLY:O	1:A:152:PRO:HD3	2.20	0.40
1:B:5:ILE:CG1	1:B:51:LEU:HB2	2.51	0.40
1:B:29:VAL:HG23	1:B:156:TRP:NE1	2.37	0.40
1:B:102:CYS:CB	1:B:116:LEU:HB3	2.51	0.40
1:A:30:ASN:N	2:A:226:HOH:O	2.55	0.40
1:A:29:VAL:C	2:A:226:HOH:O	2.60	0.40
1:A:126:ARG:CZ	1:B:96:GLY:O	2.69	0.40
1:B:84:PHE:CE1	1:B:88:MSE:HE2	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	173/237 (73%)	153 (88%)	17 (10%)	3 (2%)	<b>7</b> <b>16</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	173/237 (73%)	153 (88%)	13 (8%)	7 (4%)	2	3
All	All	346/474 (73%)	306 (88%)	30 (9%)	10 (3%)	3	6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	B	21	GLU
1	B	30	ASN
1	B	42	ASP
1	B	100	LYS
1	A	22	ARG
1	B	98	VAL
1	B	99	THR
1	B	91	GLY
1	A	58	VAL

### 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	137/203 (68%)	124 (90%)	13 (10%)	7	14
1	B	136/203 (67%)	120 (88%)	16 (12%)	4	8
All	All	273/406 (67%)	244 (89%)	29 (11%)	5	11

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	41	LEU
1	A	48	LEU
1	A	73	LEU
1	A	92	VAL
1	A	109	PRO

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	115	THR
1	A	116	LEU
1	A	138	LEU
1	A	148	LEU
1	A	153	LEU
1	A	155	GLU
1	A	172	GLU
1	B	2	LEU
1	B	14	VAL
1	B	27	ASP
1	B	36	PHE
1	B	41	LEU
1	B	48	LEU
1	B	57	LEU
1	B	62	LEU
1	B	73	LEU
1	B	115	THR
1	B	116	LEU
1	B	138	LEU
1	B	142	ARG
1	B	155	GLU
1	B	157	ARG
1	B	162	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	B	54	HIS
1	B	68	HIS
1	B	130	HIS

### 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 [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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.