



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:24 PM UTC

PDB ID : 1K3F / pdb_00001k3f
Title : Uridine Phosphorylase from E. coli, Refined in the Monoclinic Crystal Lattice
Authors : Morgunova, E.Yu.; Mikhailov, A.M.; Popov, A.N.; Blagova, E.V.; Smirnova, E.A.; Vainshtein, B.K.; Mao, C.; Armstrong, S.R.; Ealick, S.E.; Komissarov, A.A.; Linkova, E.V.; Burlakova, A.A.; Mironov, A.S.; Debabov, V.G.
Deposited on : 2001-10-02
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

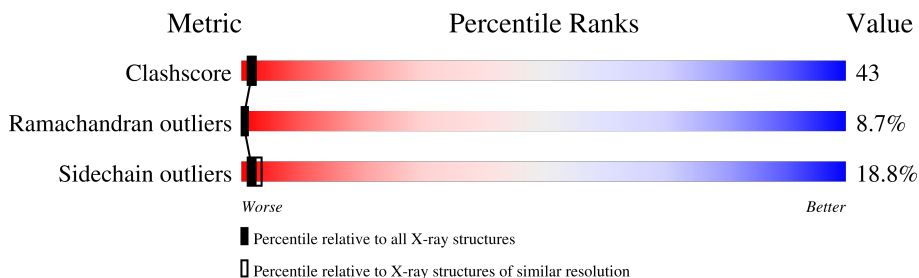
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	253	38% 43% 15% .
1	B	253	34% 44% 20% .
1	C	253	34% 46% 17% .
1	D	253	34% 43% 20% .
1	E	253	35% 43% 20% .
1	F	253	26% 52% 18% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11286 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 uridine phosphorylase.

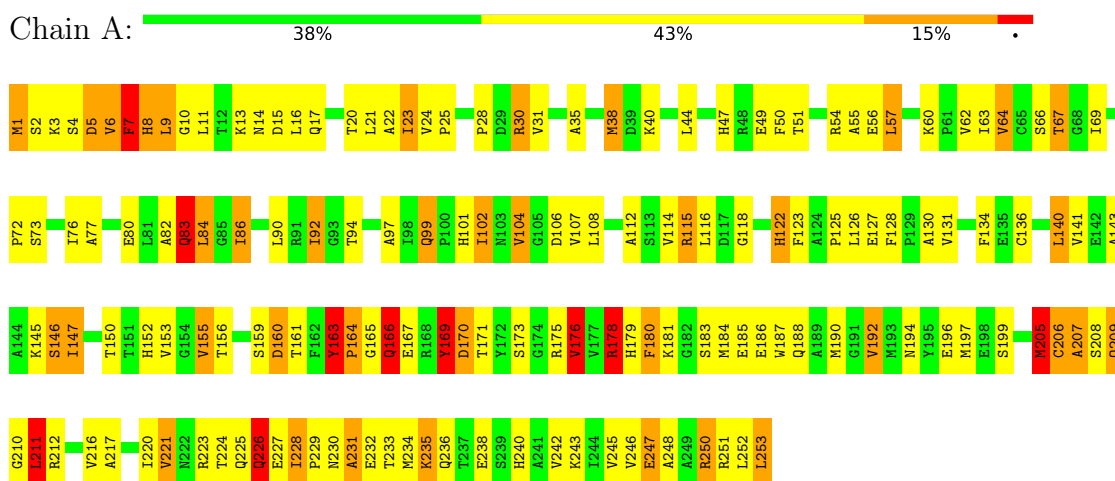
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	B	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	C	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	D	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	E	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			
1	F	253	Total	C	N	O	S	0	0	0
			1881	1180	322	367	12			

3 Residue-property plots

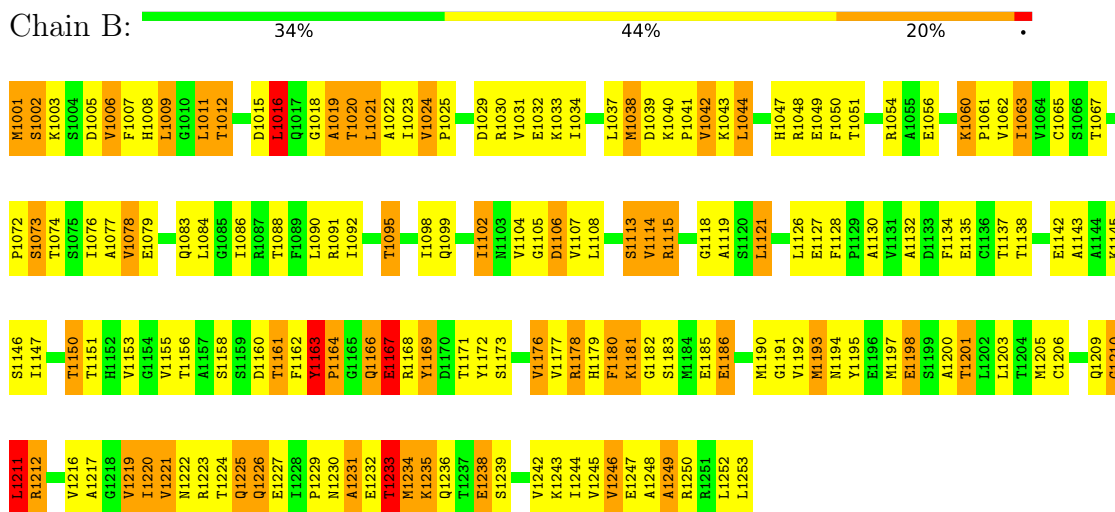
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: uridine phosphorylase

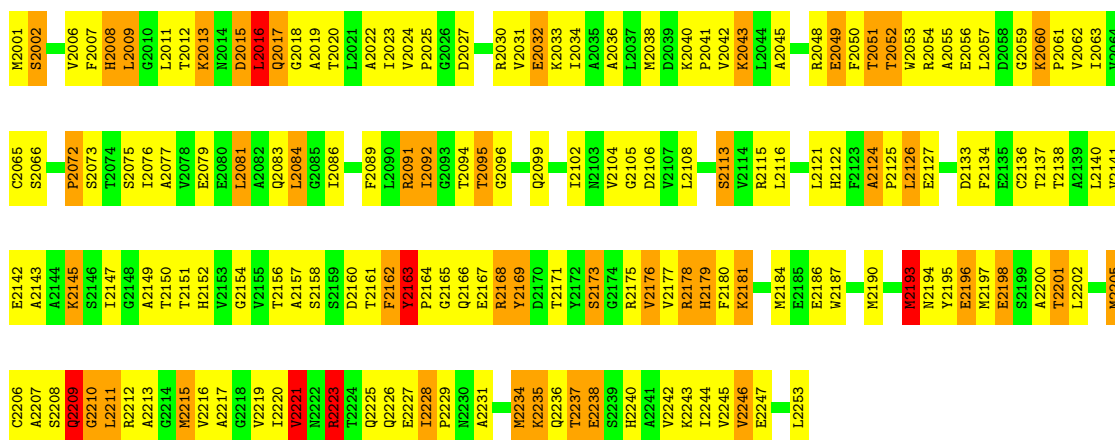


- Molecule 1: uridine phosphorylase



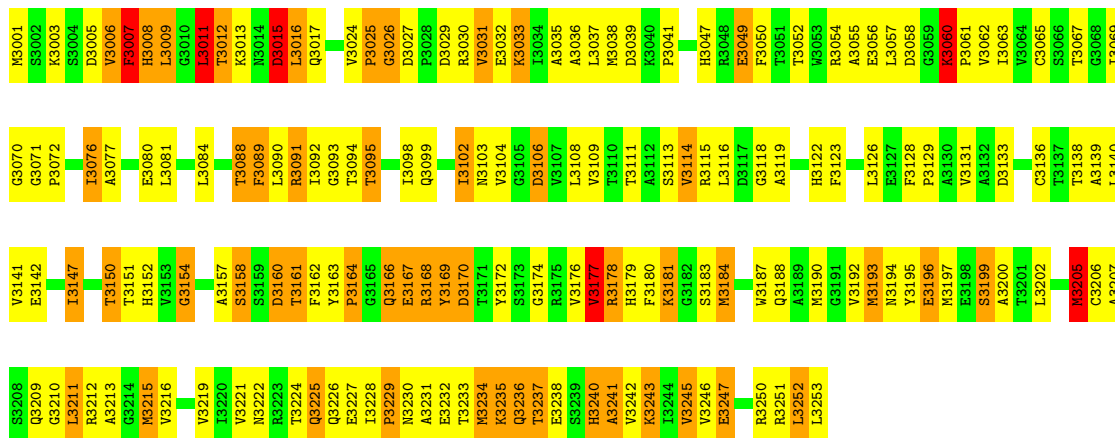
- Molecule 1: uridine phosphorylase





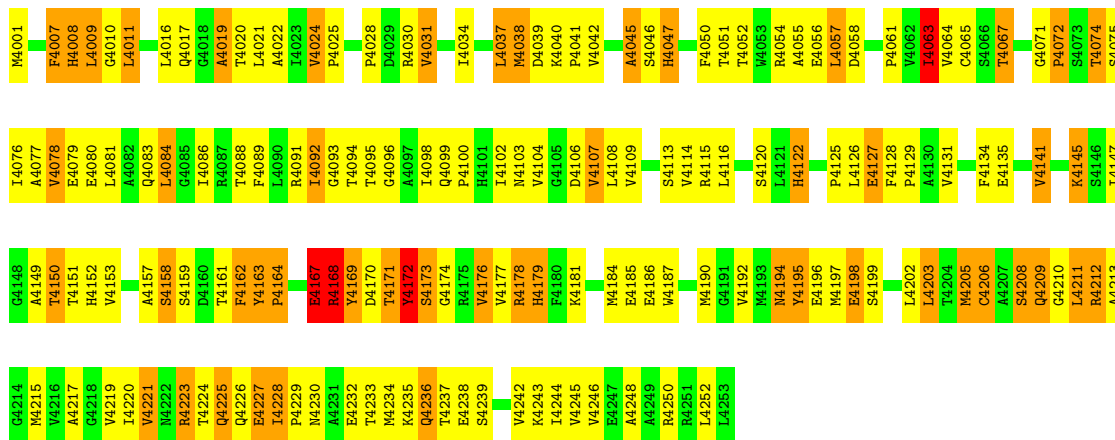
• Molecule 1: uridine phosphorylase

Chain D: 34% 43% 20% .



• Molecule 1: uridine phosphorylase

Chain E: 35% 43% 20% .



• Molecule 1: uridine phosphorylase

Chain F: 26% 52% 18% .

M5001	V5004	A5130	V5131	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194
S5002	C5065	V5131	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194	
K5003	S5066	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194		
S5004	T5067	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194		
D5005	Q5068	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194		
V5006	I5069	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194		
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A5022	F5089	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194		
I5023	L5090	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173	G5174	R5175	V5176	V5177	R5178	H5179	F5180	K5181	G5182	S5183	M5184	E5185	E5186	W5187	M5190	G5191	V5192	M5193	N5194		
V5024	R5091	A5132	D5133	F5134	E5135	C5136	T5137	T5138	A5139	L5140	V5141	E5142	A5143	A5144	K5145	S5146	I5147	H5152	V5153	G5154	V5155	T5156	A5157	S5158	S5159	D5160	T5161	F5162	Y5163	Q5166	E5167	R5168	Y5169	D5170	T5171	Y5172	S5173</																					

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.60Å 98.80Å 93.70Å 90.00° 120.20° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11286	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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	0.89	1/1913 (0.1%)	1.36	24/2599 (0.9%)
1	B	0.82	1/1913 (0.1%)	1.33	31/2599 (1.2%)
1	C	0.89	2/1913 (0.1%)	1.32	17/2599 (0.7%)
1	D	0.83	1/1913 (0.1%)	1.43	38/2599 (1.5%)
1	E	0.87	1/1913 (0.1%)	1.34	17/2599 (0.7%)
1	F	1.81	8/1913 (0.4%)	1.45	28/2599 (1.1%)
All	All	1.08	14/11478 (0.1%)	1.37	155/15594 (1.0%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	5007	PHE	CD2-CE2	29.86	2.28	1.38
1	F	5007	PHE	CD1-CE1	29.55	2.27	1.38
1	F	5007	PHE	CE1-CZ	28.52	2.24	1.38
1	F	5007	PHE	CE2-CZ	28.50	2.24	1.38
1	F	5002	SER	N-CA	23.00	1.75	1.46

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5001	MET	CA-C-N	20.03	159.80	121.54
1	F	5001	MET	C-N-CA	20.03	159.80	121.54
1	E	4170	ASP	N-CA-C	11.71	127.87	110.30
1	D	3007	PHE	N-CA-C	11.22	124.36	108.54
1	D	3027	ASP	CA-C-N	10.76	130.99	119.05

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	1881	0	1871	160	0
1	B	1881	0	1868	157	0
1	C	1881	0	1868	188	0
1	D	1881	0	1868	151	0
1	E	1881	0	1868	157	0
1	F	1881	0	1868	222	0
All	All	11286	0	11211	965	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 43.

The worst 5 of 965 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:F:5007:PHE:CD1	1:F:5007:PHE:CG	1.82	1.67
1:F:5007:PHE:CG	1:F:5007:PHE:CD2	1.83	1.60
1:F:5002:SER:N	1:F:5002:SER:CA	1.75	1.48
1:F:5007:PHE:CZ	1:F:5007:PHE:CE1	2.24	1.26
1:F:5007:PHE:CZ	1:F:5007:PHE:CE2	2.24	1.25

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	251/253 (99%)	189 (75%)	37 (15%)	25 (10%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	251/253 (99%)	180 (72%)	47 (19%)	24 (10%)	0	0
1	C	251/253 (99%)	193 (77%)	35 (14%)	23 (9%)	0	0
1	D	251/253 (99%)	194 (77%)	40 (16%)	17 (7%)	1	1
1	E	251/253 (99%)	187 (74%)	41 (16%)	23 (9%)	0	0
1	F	251/253 (99%)	193 (77%)	39 (16%)	19 (8%)	1	0
All	All	1506/1518 (99%)	1136 (75%)	239 (16%)	131 (9%)	0	0

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	PHE
1	A	13	LYS
1	A	30	ARG
1	A	163	TYR

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	200/204 (98%)	164 (82%)	36 (18%)	2	3
1	B	200/204 (98%)	161 (80%)	39 (20%)	1	2
1	C	200/204 (98%)	163 (82%)	37 (18%)	1	3
1	D	200/204 (98%)	161 (80%)	39 (20%)	1	2
1	E	200/204 (98%)	160 (80%)	40 (20%)	1	2
1	F	200/204 (98%)	166 (83%)	34 (17%)	2	4
All	All	1200/1224 (98%)	975 (81%)	225 (19%)	1	3

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3015	ASP

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Mol	Chain	Res	Type
1	F	5211	LEU
1	D	3224	THR
1	F	5202	LEU
1	F	5069	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2209	GLN
1	F	5122	HIS
1	D	3099	GLN
1	F	5240	HIS
1	E	4179	HIS

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.