



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2018 – 11:51 pm GMT

PDB ID : 1L1F
Title : Structure of human glutamate dehydrogenase-apo form
Authors : Smith, T.J.; Schmidt, T.; Fang, J.; Wu, J.; Siuzdak, G.; Stanley, C.A.
Deposited on : 2002-02-15
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

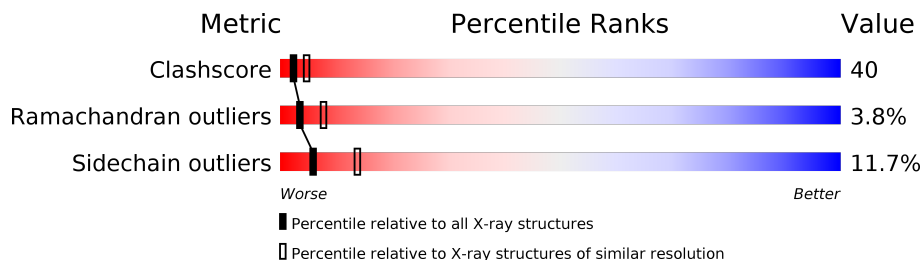
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	122078	2755 (2.70-2.70)
Ramachandran outliers	120005	2715 (2.70-2.70)
Sidechain outliers	119972	2715 (2.70-2.70)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	
1	C	505	
1	D	505	
1	E	505	
1	F	505	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23244 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 Glutamate Dehydrogenase 1.

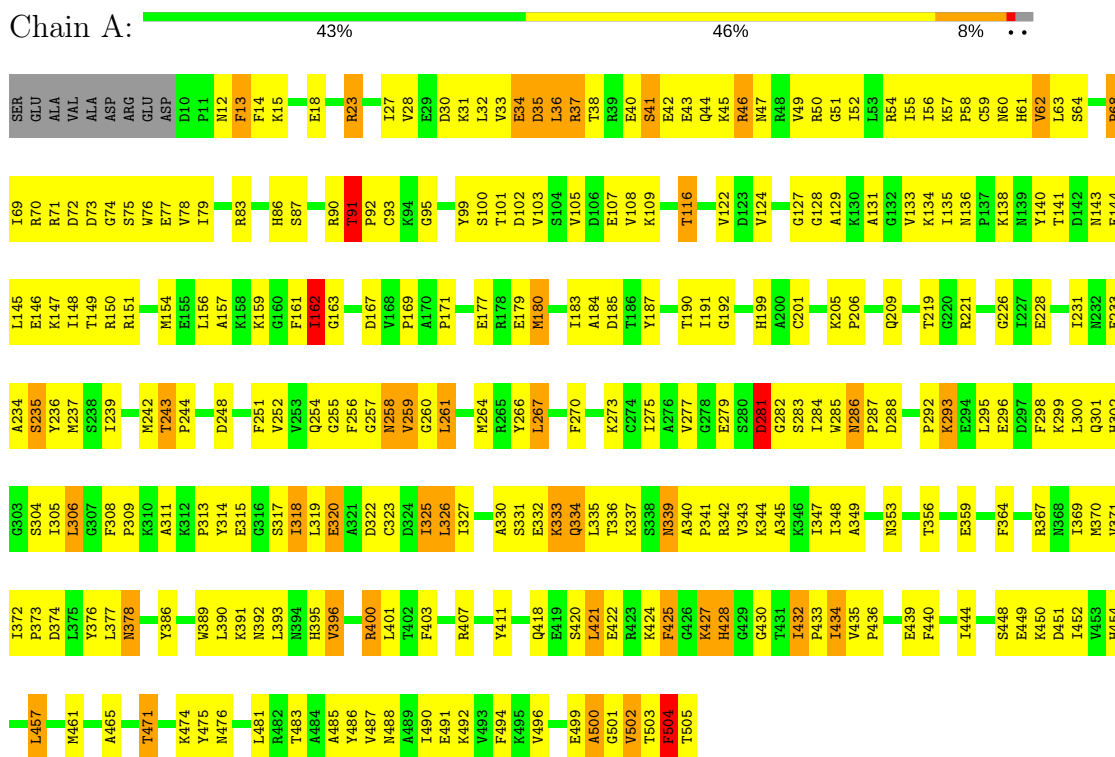
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			

3 Residue-property plots

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 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.

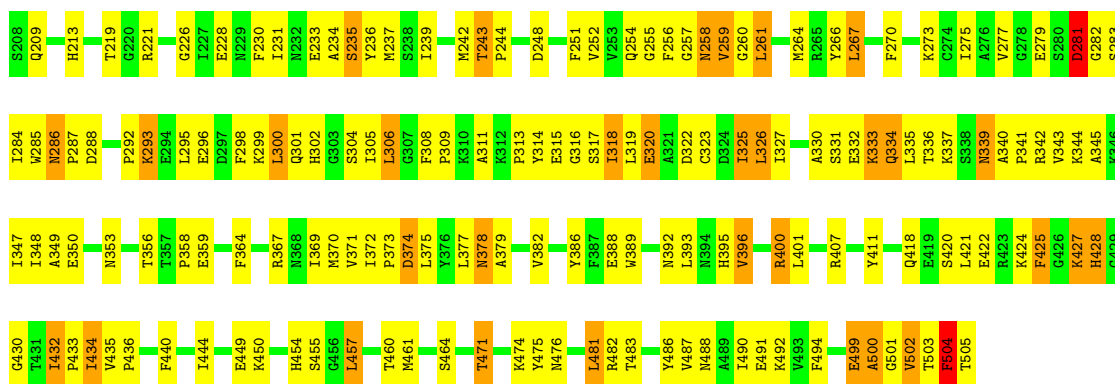
Note EDS was not executed.

• Molecule 1: Glutamate Dehydrogenase 1



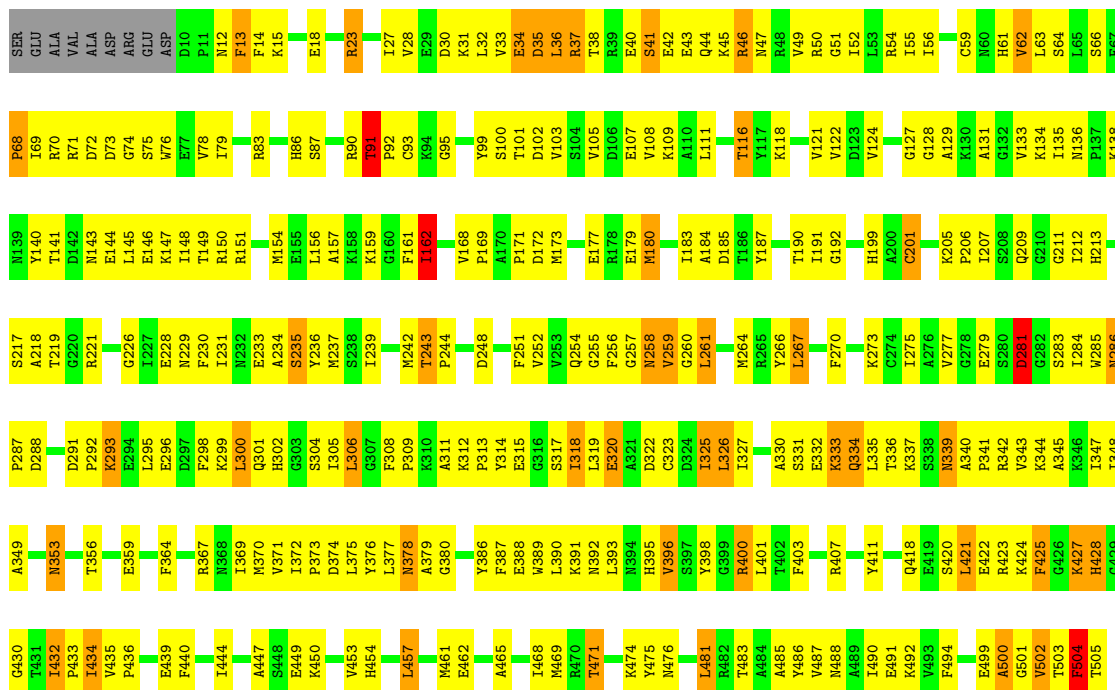
• Molecule 1: Glutamate Dehydrogenase 1





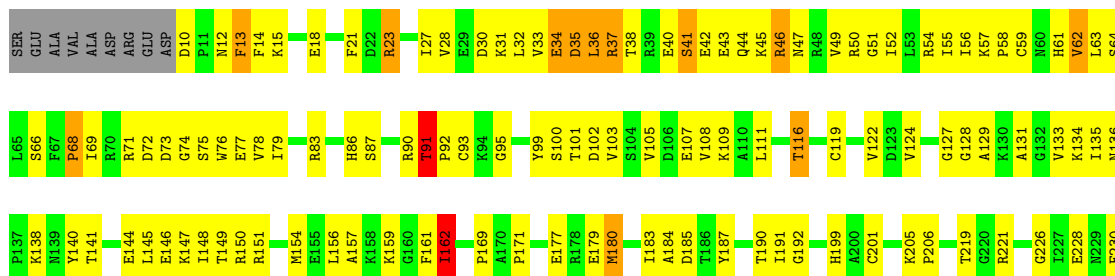
• Molecule 1: Glutamate Dehydrogenase 1

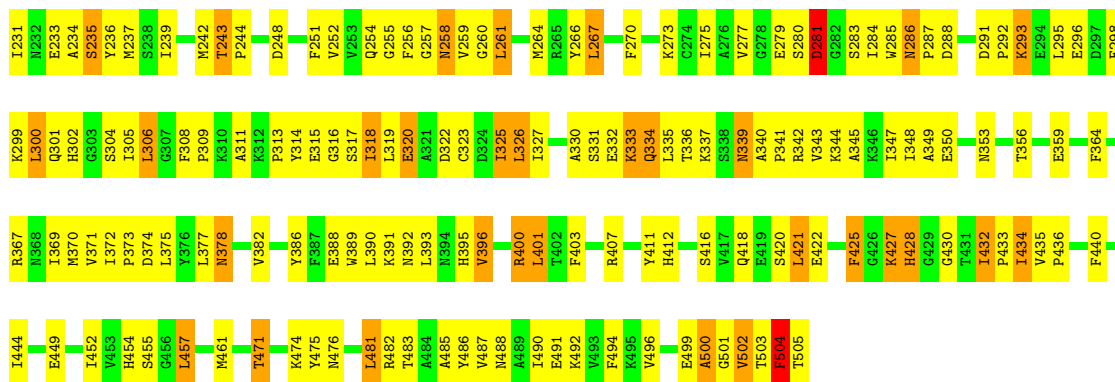
Chain C: 40% 49% 9% ..



• Molecule 1: Glutamate Dehydrogenase 1

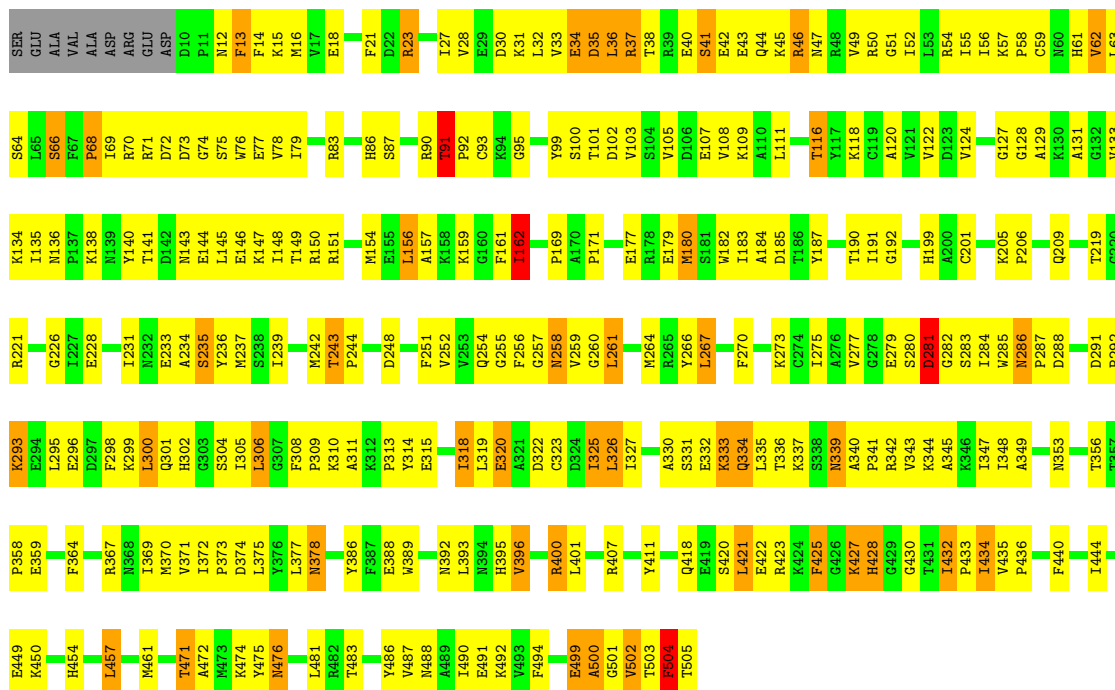
Chain D: 43% 46% 9% ..





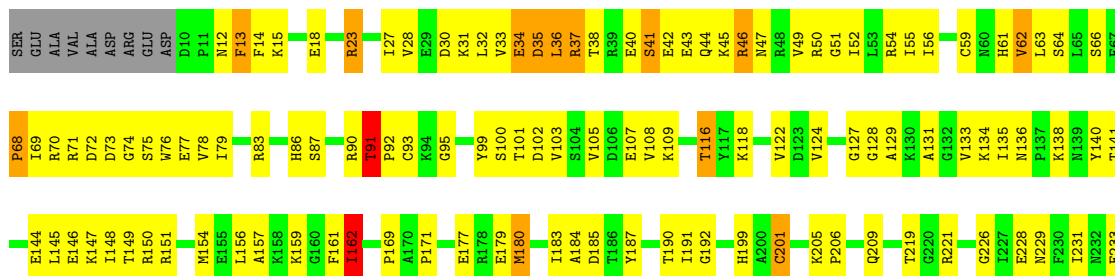
• Molecule 1: Glutamate Dehydrogenase 1

Chain E: 43% 45% 9% ..



• Molecule 1: Glutamate Dehydrogenase 1

Chain F: 43% 46% 8% ..



A234	G303	V371	H454
S235	S304	I372	L457
Y236	I305	D373	E462
M237	L306	P374	R463
G238	G307	Y375	S464
L239	F308	Y376	A465
M242	P309	L377	T471
T243	K310	N378	K474
P244	A311	A379	Y475
D248	P312	Y386	M476
P251	P313	Y389	L481
V252	Y314	L390	R482
V253	E315	K391	T483
Q254	G316	N392	A484
G255	S317	L393	A485
P256	I318	N394	Y486
G257	L319	H395	V487
M258	E320	V396	N488
G260	A321	R400	A489
L261	D322	L401	I490
M264	C323	T402	E491
R265	I325	F403	V493
Y266	I326	R407	F494
L267	I327	Y411	E499
F270	P328	Q418	A500
K273	A329	E419	G501
C274	A330	S420	V502
I275	S331	L421	T503
A276	E332	E422	F504
V277	K333	R423	T505
G278	S338	K424	
E279	A340	F425	
S280	P341	G426	
D281	R342	K427	
G282	V343	H428	
S283	K344	G429	
I284	A345	G430	
M285	K346	T431	
N286	I347	I432	
P287	I348	P433	
D288	A349	I434	
P292	N353	V435	
K293	T356	P436	
E294	E359	E439	
E296	F364	F440	
D297	R367	I444	
F298	N368	A447	
K299	I369	S448	
L300	M370	E449	
Q301		K450	
H302			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.80Å 98.80Å 124.20Å 86.26° 70.28° 60.34°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program		Depositor
R, R_{free}	0.262 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23244	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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	0.62	1/3958 (0.0%)	0.82	3/5340 (0.1%)
1	B	0.63	1/3958 (0.0%)	0.82	5/5340 (0.1%)
1	C	0.65	2/3958 (0.1%)	0.82	4/5340 (0.1%)
1	D	0.62	1/3958 (0.0%)	0.82	5/5340 (0.1%)
1	E	0.62	1/3958 (0.0%)	0.82	4/5340 (0.1%)
1	F	0.62	2/3958 (0.1%)	0.82	5/5340 (0.1%)
All	All	0.63	8/23748 (0.0%)	0.82	26/32040 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	CYS	CB-SG	8.91	1.97	1.82
1	C	59	CYS	CB-SG	8.33	1.96	1.82
1	A	59	CYS	CB-SG	7.79	1.95	1.82
1	B	59	CYS	CB-SG	7.48	1.95	1.82
1	F	201	CYS	CB-SG	-7.10	1.70	1.82

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	504	PHE	N-CA-C	-7.28	91.34	111.00
1	C	504	PHE	N-CA-C	-7.28	91.35	111.00
1	B	504	PHE	N-CA-C	-7.27	91.38	111.00
1	F	504	PHE	N-CA-C	-7.25	91.43	111.00
1	D	504	PHE	N-CA-C	-7.19	91.60	111.00

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	3874	0	3841	316	0
1	B	3874	0	3841	333	0
1	C	3874	0	3841	366	0
1	D	3874	0	3841	326	0
1	E	3874	0	3841	341	0
1	F	3874	0	3841	324	0
All	All	23244	0	23046	1865	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 40.

The worst 5 of 1865 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:C:285:TRP:HB2	1:C:314:TYR:HB2	1.31	1.13
1:E:285:TRP:HB2	1:E:314:TYR:HB2	1.30	1.12
1:F:285:TRP:HB2	1:F:314:TYR:HB2	1.29	1.09
1:A:285:TRP:HB2	1:A:314:TYR:HB2	1.30	1.08
1:B:285:TRP:HB2	1:B:314:TYR:HB2	1.29	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3	8
1	C	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3	8
1	D	494/505 (98%)	426 (86%)	49 (10%)	19 (4%)	3	8
1	E	494/505 (98%)	425 (86%)	50 (10%)	19 (4%)	3	8
1	F	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3	8
All	All	2964/3030 (98%)	2563 (86%)	287 (10%)	114 (4%)	3	8

5 of 114 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	41	SER
1	A	91	THR
1	A	102	ASP
1	A	258	ASN

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	413/420 (98%)	365 (88%)	48 (12%)	6	14
1	B	413/420 (98%)	364 (88%)	49 (12%)	6	13
1	C	413/420 (98%)	365 (88%)	48 (12%)	6	14
1	D	413/420 (98%)	364 (88%)	49 (12%)	6	13
1	E	413/420 (98%)	365 (88%)	48 (12%)	6	14
1	F	413/420 (98%)	365 (88%)	48 (12%)	6	14
All	All	2478/2520 (98%)	2188 (88%)	290 (12%)	6	14

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	378	ASN

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Mol	Chain	Res	Type
1	D	235	SER
1	F	315	GLU
1	C	421	LEU
1	D	36	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	410	ASN
1	D	378	ASN
1	F	378	ASN
1	C	488	ASN
1	D	86	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 ⓘ

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

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.