



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:31 PM UTC

PDB ID : 1L1F / pdb_0000111f
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 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

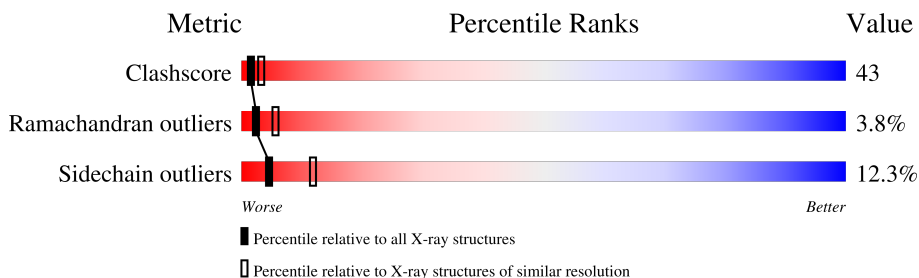
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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	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.

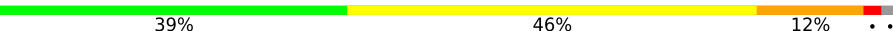
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3874	2450	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
	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

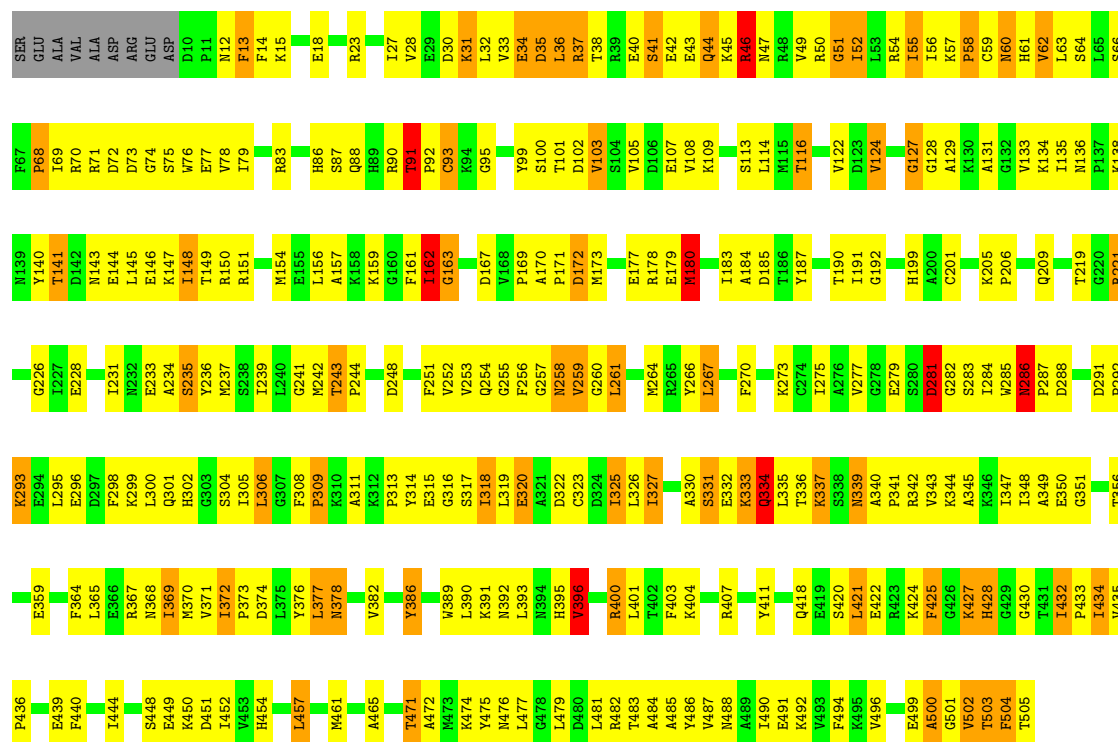
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

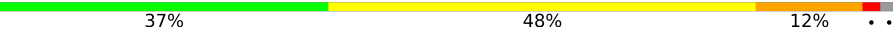
Note EDS was not executed.

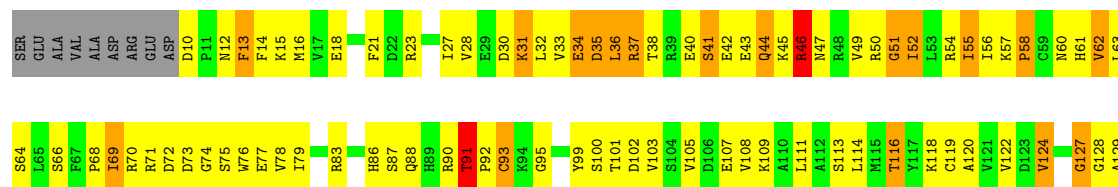
• Molecule 1: Glutamate Dehydrogenase 1

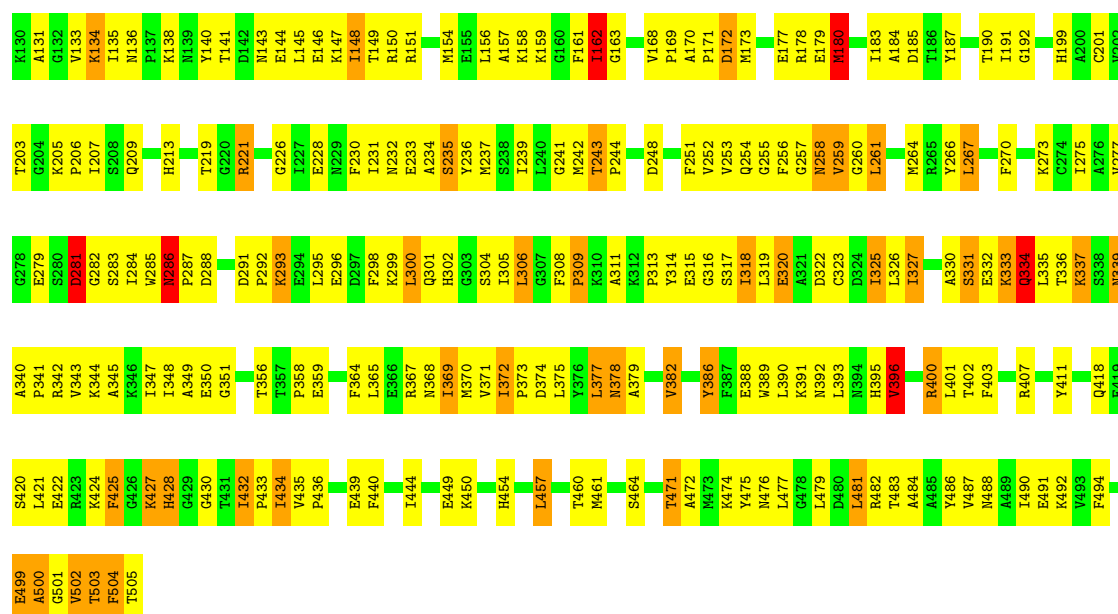
Chain A: 



• Molecule 1: Glutamate Dehydrogenase 1

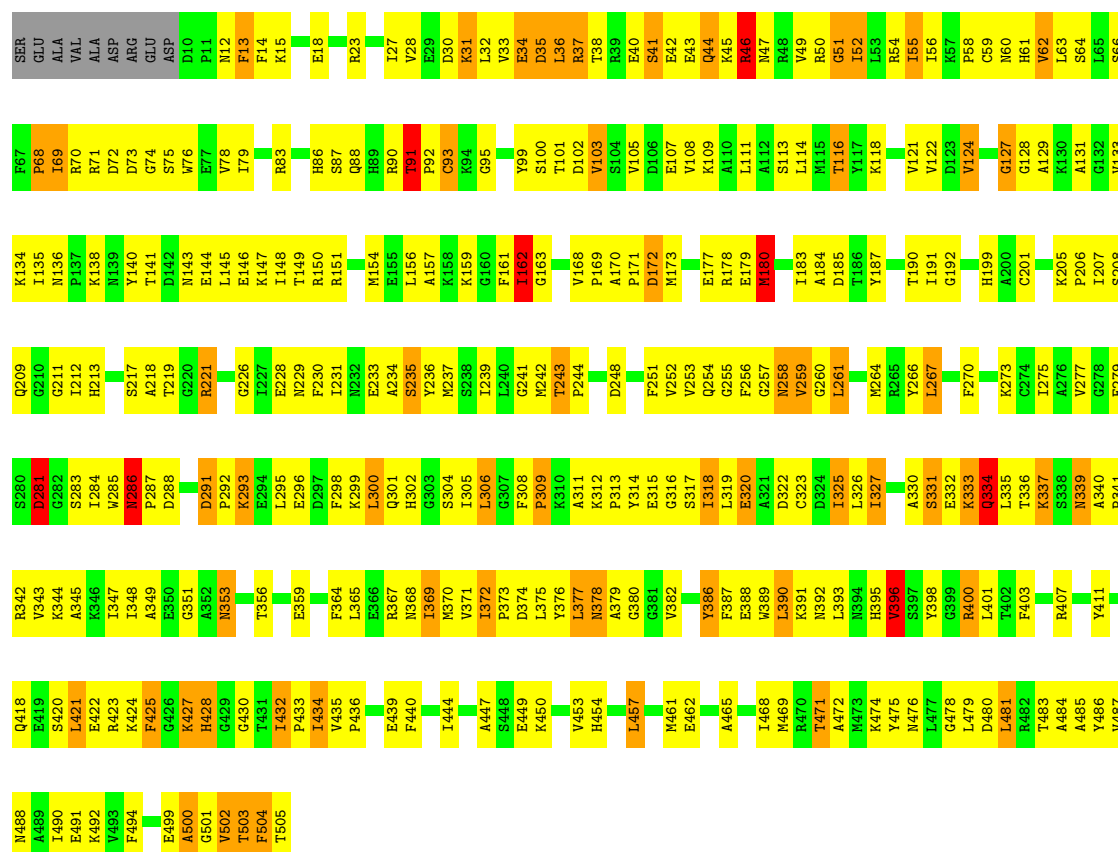
Chain B: 



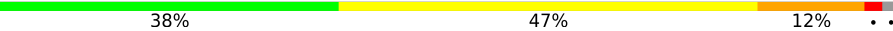


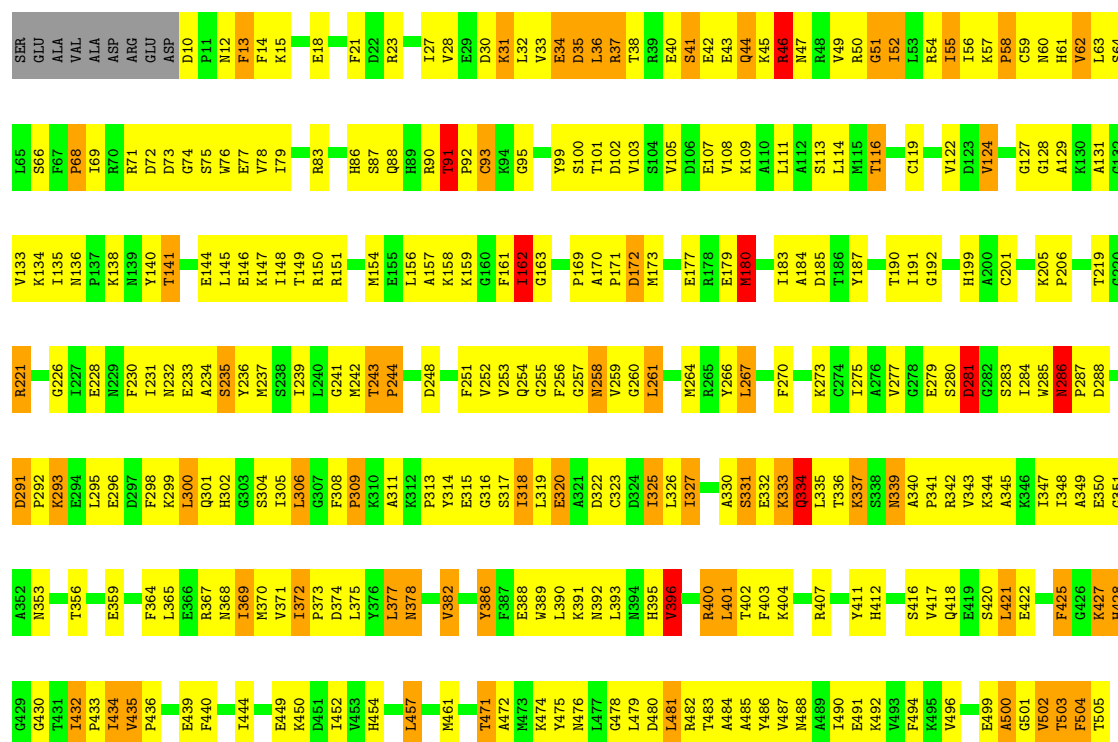
• Molecule 1: Glutamate Dehydrogenase 1

Chain C: 35% 49% 12% ..



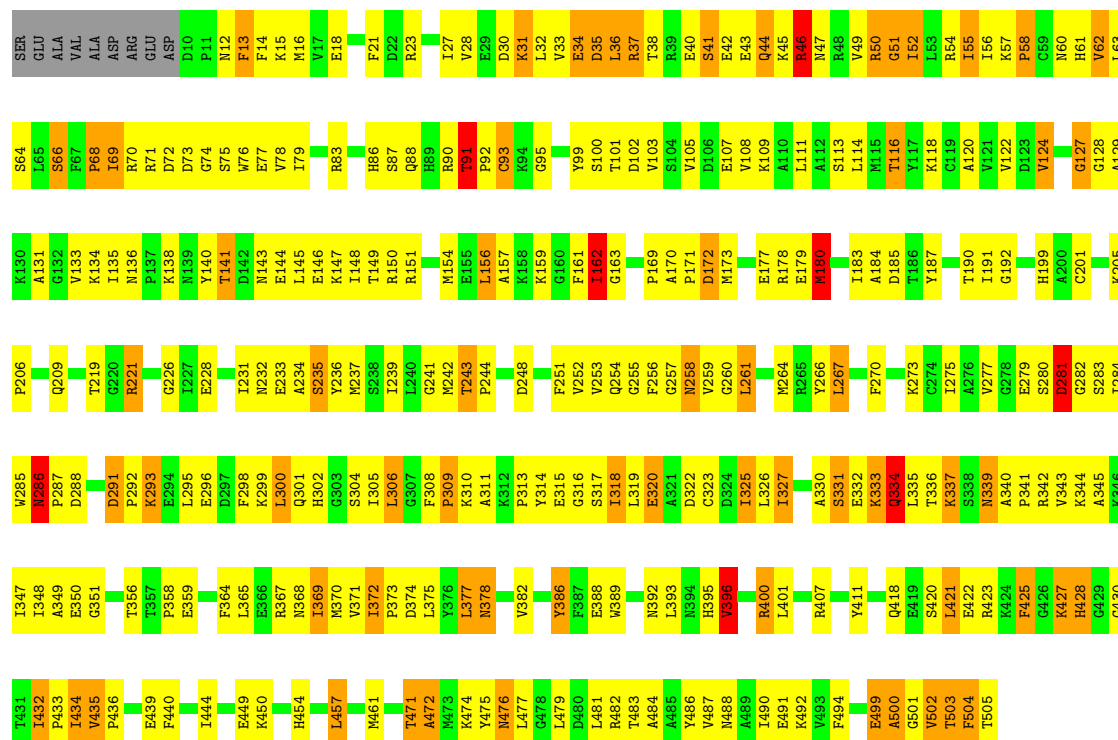
• Molecule 1: Glutamate Dehydrogenase 1

Chain D:  38% 47% 12% ..



• Molecule 1: Glutamate Dehydrogenase 1

Chain E:  39% 45% 13% ..



• Molecule 1: Glutamate Dehydrogenase 1

Chain F: 

P433	N353	K293	G226	P137	F67	SER
I434	E294	E294	I227	K138	P68	GLU
V435	T356	L295	E228	N139	I69	ALA
P436	E296	E296	N229	Y140	VAL	VAL
E439	E359	D297	F230	T141	R71	ALA
		F298	I231		D72	ASP
F440	F364	K299	N232	E144	D73	ARG
	L365	L300	E233	L145	GLU	GLU
I444	E366	Q301	A234	S75	ASP	ASP
A447	R367	H302	S235	K147	W76	D10
S448	N368	G303	Y236	T148	E77	P11
E449	I369	S304	M237	T149	V78	N12
K450	M370	I305	S238	R150	I79	F13
H454	V371	L306	T239	R151	F14	F14
	I372	G307	L240		R83	K15
L457	P373	F308	G241	M154		E18
	D374	P309	M242	L155	H86	
	L375	K310	T243	L156	S87	R23
	Y376	A311	P244	A157	Q88	
E462	L377	K312		K158	H89	
R463	N378	P313	D248	K159	R90	L27
S464	A379	Y314		G160	T91	V28
A465		E315	F251	F161	P92	E99
	V382	G316	V252	I162	C93	D30
		S317	V253	G163	R31	
M469	Y386	T318	Q254	R94	C95	L32
R470	L319	L318	G255	P169	V33	
T471	E320	F256	N258	A170	Y99	E34
M473	A321	G257	D172	P171	S100	D35
K474	D322	C323	M173	D172	T101	L36
Y475	N392	D324		E177	D102	R37
L477	L393	G326		V103	T38	
G478	N394	I325	L261	R178	R39	R39
L479	H395	L326	M264	E178	V105	E40
	Y386	P327	R265	E179	D106	S41
D480		R328	R266	H180	E107	E42
L481	R400	A329	V266	I183	V108	E43
R482	L401	A330	L267	A184	K109	Q44
T483	T402	S331		D185	K45	
A484	F403	E332	F270	T186	S113	R46
A485	K333	K333		Y187	L114	N47
Y486	R407	Q334	K273		M115	R48
V487		L335	C274		T116	V49
M488	Y411	T336	L275		Y117	R50
A489		K337	A276		K118	
I490	Q418	S338	V277	G192		I52
E491	E419	N339	G278	V122	L53	R54
K492	S420	A340	E279	H199	D123	
V493	L421	P341	S260	A200	V124	I56
F494	E422	R342	D281	C201		R57
	R423	V343	G282	K205	G127	P58
E499	K424	K344	S283	P206	A129	C59
A500	F425	A345	I284		K130	N60
G501	G426	K346	V285	Q209	A131	H61
V502	K427	I347	R286	G132		V62
T503	H428	T348	P287	V133	K134	L63
F504	G429	A349	D288	T219	I135	S64
T505	G430	E350	D291	G220	L65	
		G351	D291	R221		S66
	I432	A352	P292			

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	0.75	1/3958 (0.0%)	1.25	47/5340 (0.9%)
1	B	0.80	1/3958 (0.0%)	1.26	49/5340 (0.9%)
1	C	0.81	1/3958 (0.0%)	1.26	50/5340 (0.9%)
1	D	0.78	1/3958 (0.0%)	1.26	48/5340 (0.9%)
1	E	0.79	1/3958 (0.0%)	1.26	50/5340 (0.9%)
1	F	0.77	1/3958 (0.0%)	1.25	46/5340 (0.9%)
All	All	0.78	6/23748 (0.0%)	1.26	290/32040 (0.9%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	MET	SD-CE	-9.28	1.56	1.79
1	F	180	MET	SD-CE	-8.39	1.58	1.79
1	B	180	MET	SD-CE	-7.49	1.60	1.79
1	E	180	MET	SD-CE	-7.32	1.61	1.79
1	A	180	MET	SD-CE	-7.25	1.61	1.79

The worst 5 of 290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	504	PHE	N-CA-C	-15.33	91.34	110.65
1	C	504	PHE	N-CA-C	-15.32	91.35	110.65
1	B	504	PHE	N-CA-C	-15.29	91.38	110.65
1	F	504	PHE	N-CA-C	-15.26	91.43	110.65
1	D	504	PHE	N-CA-C	-15.12	91.60	110.65

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	3874	0	3841	335	0
1	B	3874	0	3841	348	0
1	C	3874	0	3841	382	0
1	D	3874	0	3841	349	0
1	E	3874	0	3841	358	0
1	F	3874	0	3841	345	0
All	All	23244	0	23046	1971	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 1971 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 [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	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2	5
1	C	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2	5
1	D	494/505 (98%)	426 (86%)	49 (10%)	19 (4%)	2	5
1	E	494/505 (98%)	425 (86%)	50 (10%)	19 (4%)	2	5
1	F	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	2	5
All	All	2964/3030 (98%)	2563 (86%)	287 (10%)	114 (4%)	2	5

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%)	362 (88%)	51 (12%)	4	12
1	B	413/420 (98%)	363 (88%)	50 (12%)	5	12
1	C	413/420 (98%)	361 (87%)	52 (13%)	4	11
1	D	413/420 (98%)	361 (87%)	52 (13%)	4	11
1	E	413/420 (98%)	363 (88%)	50 (12%)	5	12
1	F	413/420 (98%)	363 (88%)	50 (12%)	5	12
All	All	2478/2520 (98%)	2173 (88%)	305 (12%)	4	12

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	306	LEU

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Mol	Chain	Res	Type
1	F	326	LEU
1	E	334	GLN
1	F	46	ARG
1	F	457	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	302	HIS
1	E	86	HIS
1	F	410	ASN
1	D	353	ASN
1	D	467	GLN

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.