wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 02:51 am BST

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

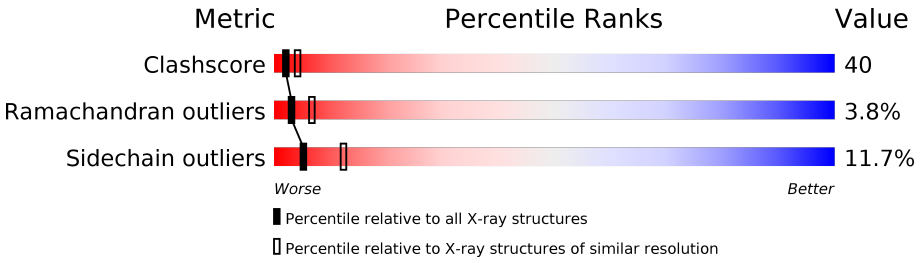
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	505	43% 46% 8%
1	B	505	41% 48% 9%
1	C	505	40% 49% 9%
1	D	505	43% 46% 9%
1	E	505	43% 45% 9%
1	F	505	43% 46% 8%

2 Entry composition (i)

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			

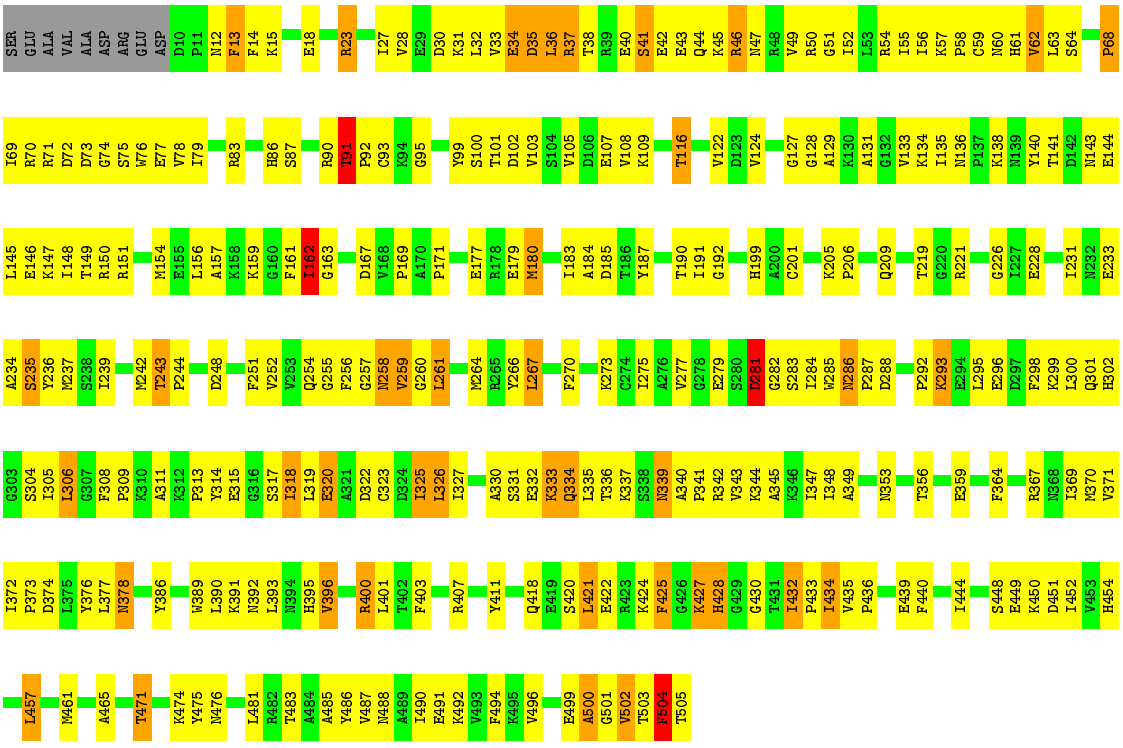
3 Residue-property plots (i)

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.

Note EDS was not executed.

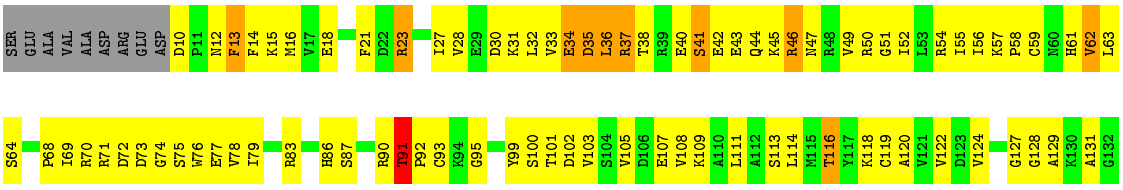
- Molecule 1: Glutamate Dehydrogenase 1

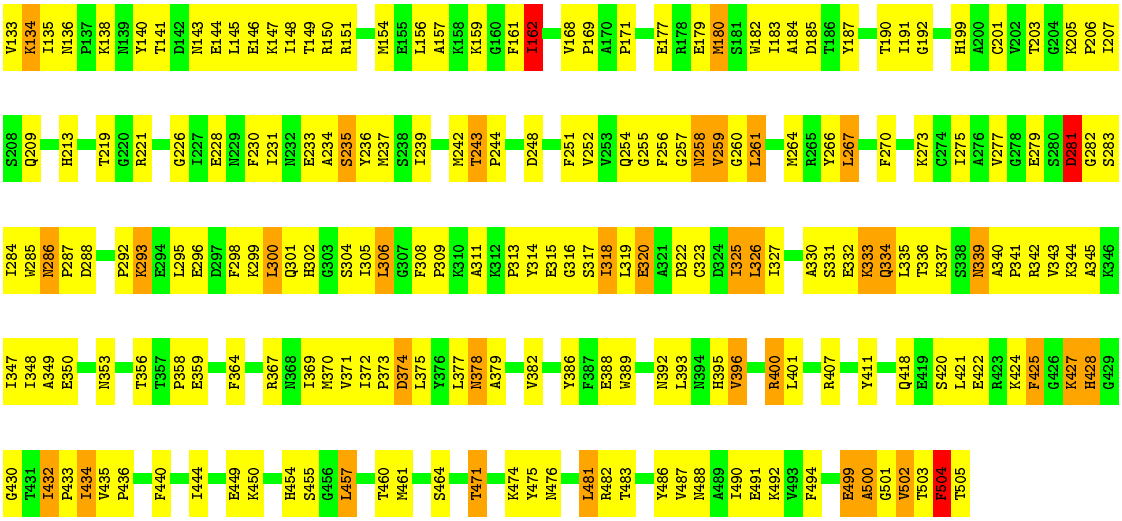
Chain A:



- Molecule 1: Glutamate Dehydrogenase 1

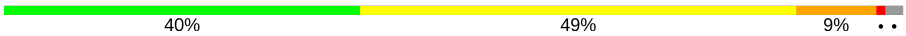
Chain B:

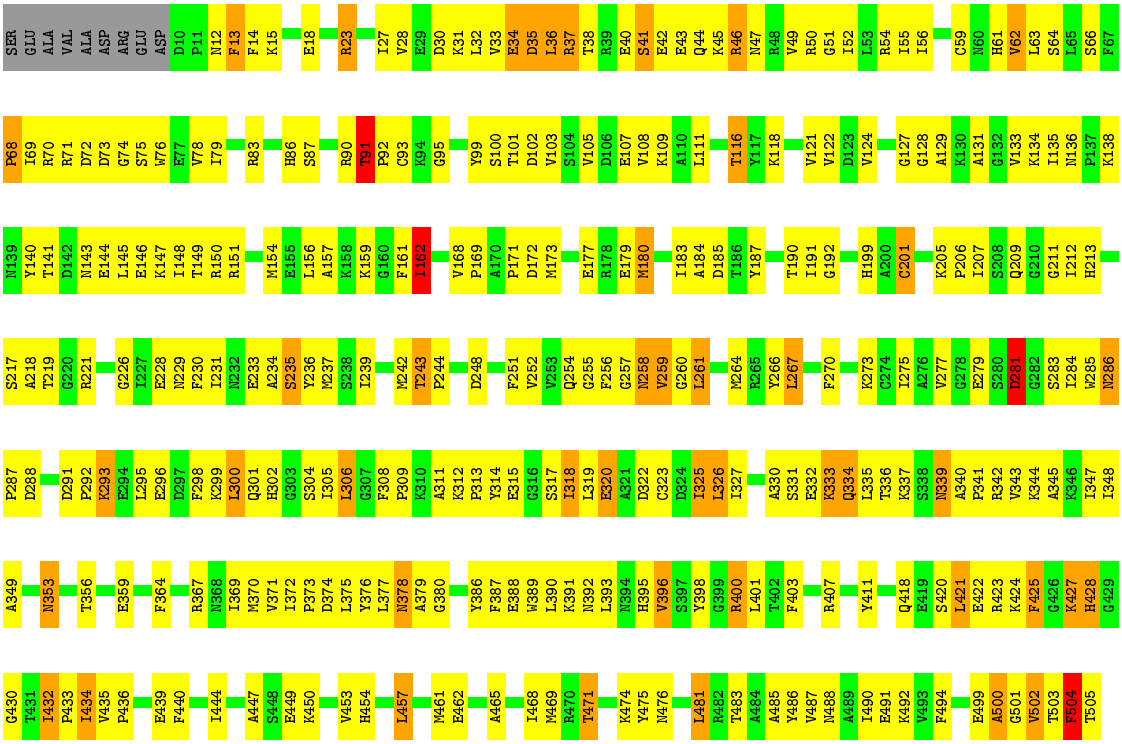




• Molecule 1: Glutamate Dehydrogenase 1

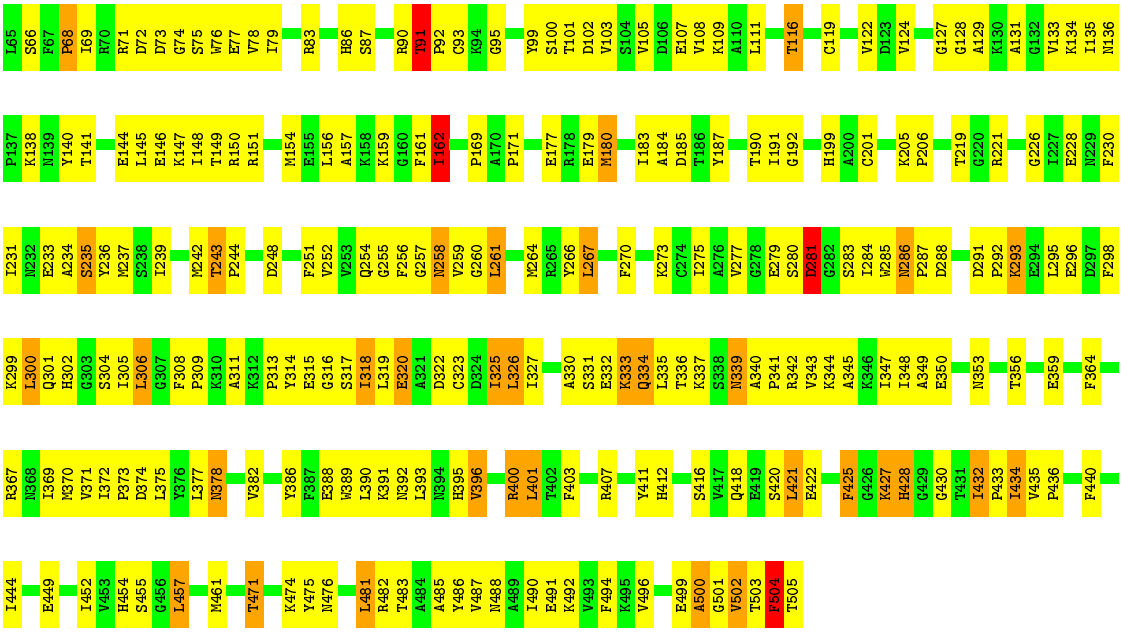
Chain C:





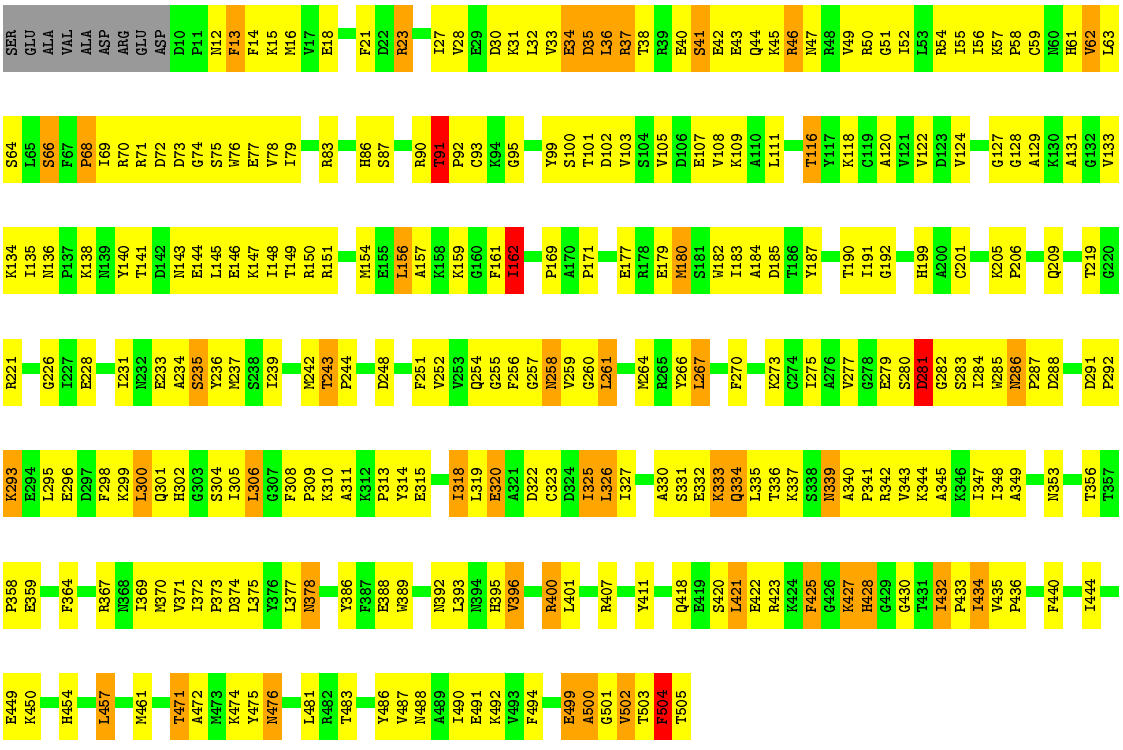
• Molecule 1: Glutamate Dehydrogenase 1

Chain D:



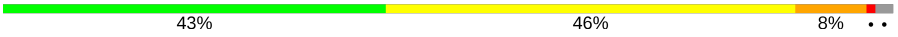
• Molecule 1: Glutamate Dehydrogenase 1

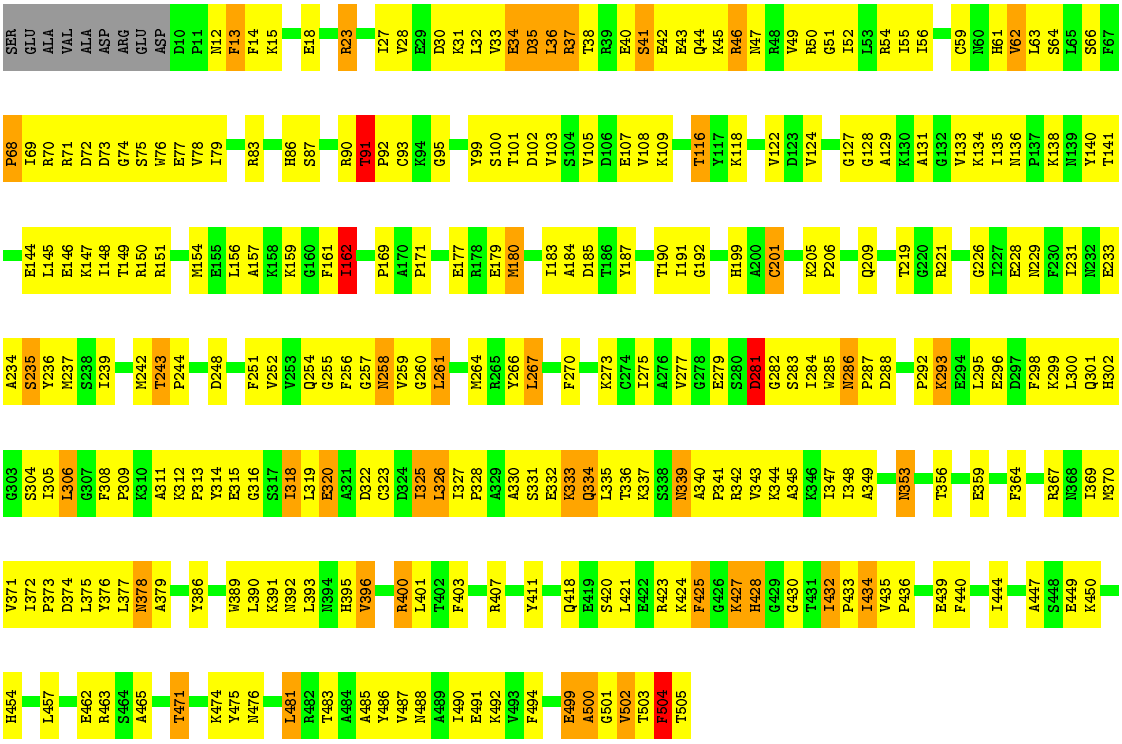
Chain E:



• Molecule 1: Glutamate Dehydrogenase 1

Chain F:




SER GLU ALA VAL ALA ASP ARG GLU ASP D10 P11 N12 F13 F14 K15 E18 R23 I27 V28 E29 D30 K31 L32 V33 E34 D35 L36 R37 T38 R39 E40 S41 E42 E43 Q44 K45 R46 M47 R48 V49 R50 G51 I52 L53 R54 I55 I56 C59 N60 H61 V62 L63 S64 L65 S66 F67
P68 I69 R70 R71 D72 D73 G74 S75 W76 E77 V78 I79 R83 H86 S87 R90 T91 P92 C93 K94 G95 Y99 S100 T101 D102 V103 S104 V105 D106 E107 V108 K109 T116 Y117 K118 V122 D123 V124 G127 G128 A129 K130 A131 G132 V133 K134 I135 N136 P137 K138 N139 Y140 T141
E144 L145 E146 K147 I148 T149 R150 R151 M154 E155 L156 A157 K158 K159 G160 F161 I162 P169 A170 P171 E177 R178 E179 M180 I183 A184 D185 T186 Y187 T190 I191 G192 H199 A200 C201 K205 P206 Q209 T219 G220 R221 G226 I227 E228 N229 F230 I231 N232 E233
A234 S235 Y236 M237 S238 I239 M242 T243 P244 D248 F251 V252 V253 Q254 G255 F256 G257 N258 V259 G260 L261 M264 R265 Y266 L267 F270 K273 C274 I275 A276 V277 G278 E279 S280 D281 G282 S283 I284 W285 N286 P287 D288 P292 K293 E294 L295 E296 D297 F298 K299 L300 Q301 H302
G303 S304 I305 L306 G307 F308 P309 K310 A311 K312 P313 Y314 E315 G316 S317 I318 L319 E320 A321 D322 C323 D324 I325 L326 I327 P328 A329 A330 S331 E332 K333 Q334 L335 T336 K337 S338 N339 A340 P341 R342 V343 K344 A345 K346 I347 I348 A349 N353 T356 E359 F364 R367 N368 I369 M370
V371 I372 P373 D374 L375 Y376 L377 N378 A379 Y386 W389 L390 K391 N392 L393 N394 H395 V396 R400 L401 T402 F403 R407 Y411 Q418 E419 S420 L421 E422 R423 K424 F425 G426 K427 H428 G429 G430 T431 I432 P433 I434 V435 P436 E439 F440 I444 A447 S448 E449 K450
H454 L457 E462 R463 S464 A465 T471 K474 Y475 N476 L481 R482 T483 A484 A485 Y486 V487 N488 A489 I490 E491 K492 V493 F494 E499 A500 G501 V502 T503 F504 T505

4 Data and refinement statistics (i)

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

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	0.62	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(^{o})	Ideal(^{o})
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 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3 7
1	C	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3 7
1	D	494/505 (98%)	426 (86%)	49 (10%)	19 (4%)	3 7
1	E	494/505 (98%)	425 (86%)	50 (10%)	19 (4%)	3 7
1	F	494/505 (98%)	428 (87%)	47 (10%)	19 (4%)	3 7
All	All	2964/3030 (98%)	2563 (86%)	287 (10%)	114 (4%)	3 7

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%)	5 12
1	B	413/420 (98%)	364 (88%)	49 (12%)	5 12
1	C	413/420 (98%)	365 (88%)	48 (12%)	5 12
1	D	413/420 (98%)	364 (88%)	49 (12%)	5 12
1	E	413/420 (98%)	365 (88%)	48 (12%)	5 12
1	F	413/420 (98%)	365 (88%)	48 (12%)	5 12
All	All	2478/2520 (98%)	2188 (88%)	290 (12%)	5 12

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 (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 carbohydrates 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.