



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:30 PM UTC

PDB ID : 1BVU / pdb_00001bvu
Title : GLUTAMATE DEHYDROGENASE FROM THERMOCOCCUS LITORALIS
Authors : Baker, P.J.; Britton, K.L.; Yip, K.S.; Stillman, T.J.; Rice, D.W.
Deposited on : 1999-07-20
Resolution : 2.50 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

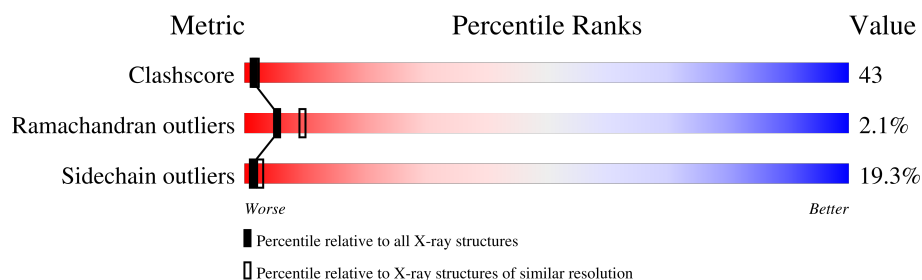
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	418	32% 50% 16% .
1	B	418	38% 50% 11% .
1	C	418	39% 44% 15% .
1	D	418	35% 46% 17% .
1	E	418	37% 49% 12% .
1	F	418	38% 48% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19566 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 PROTEIN (GLUTAMATE DEHYDROGENASE).

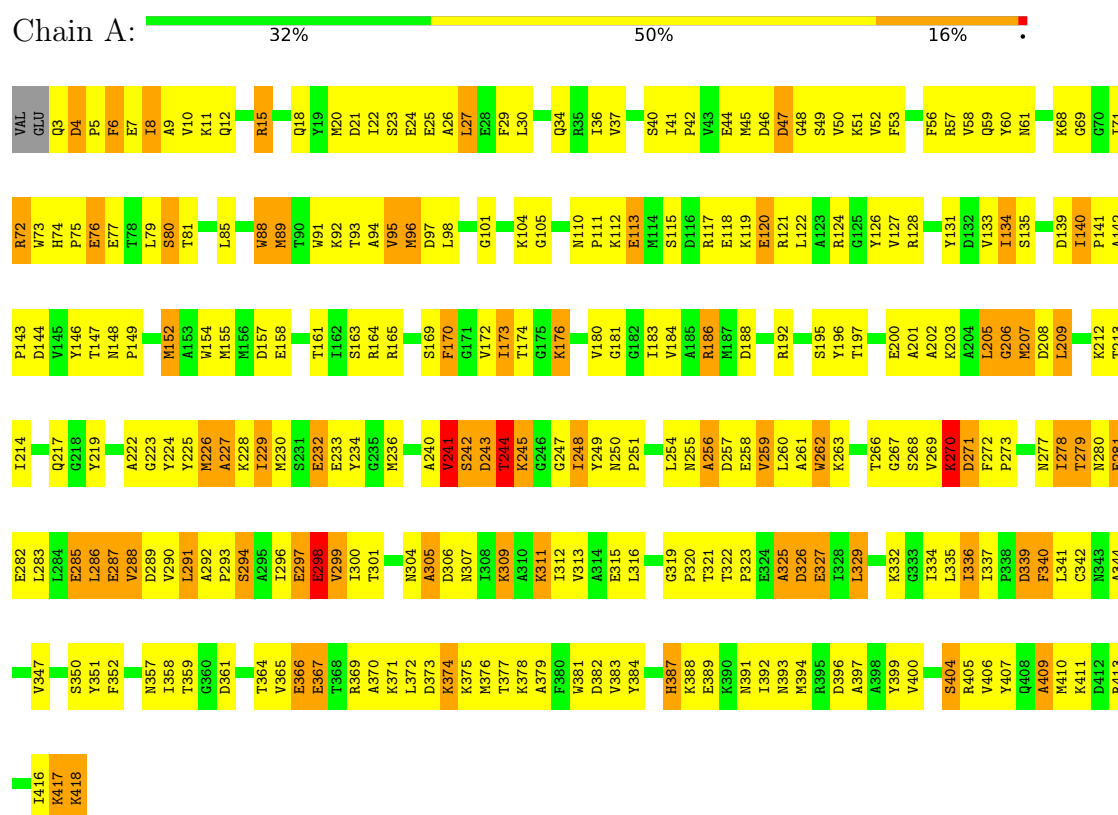
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	B	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	C	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	D	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	E	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	F	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			

3 Residue-property plots

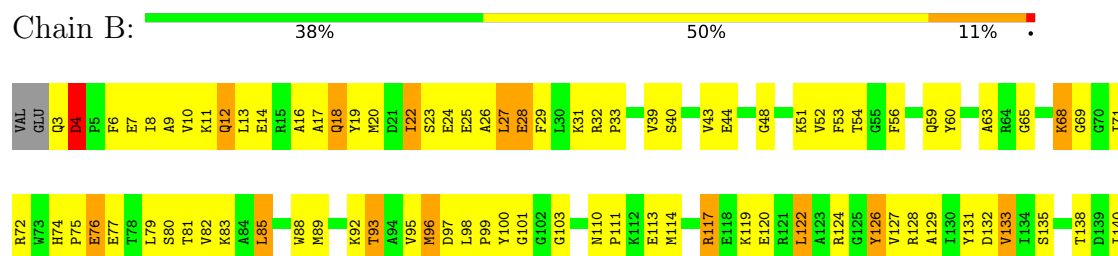
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

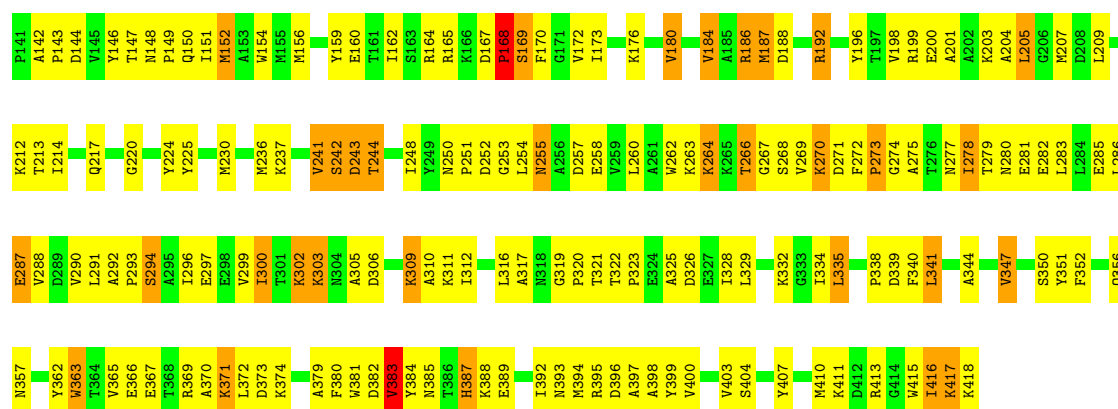
Note EDS was not executed.

• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)



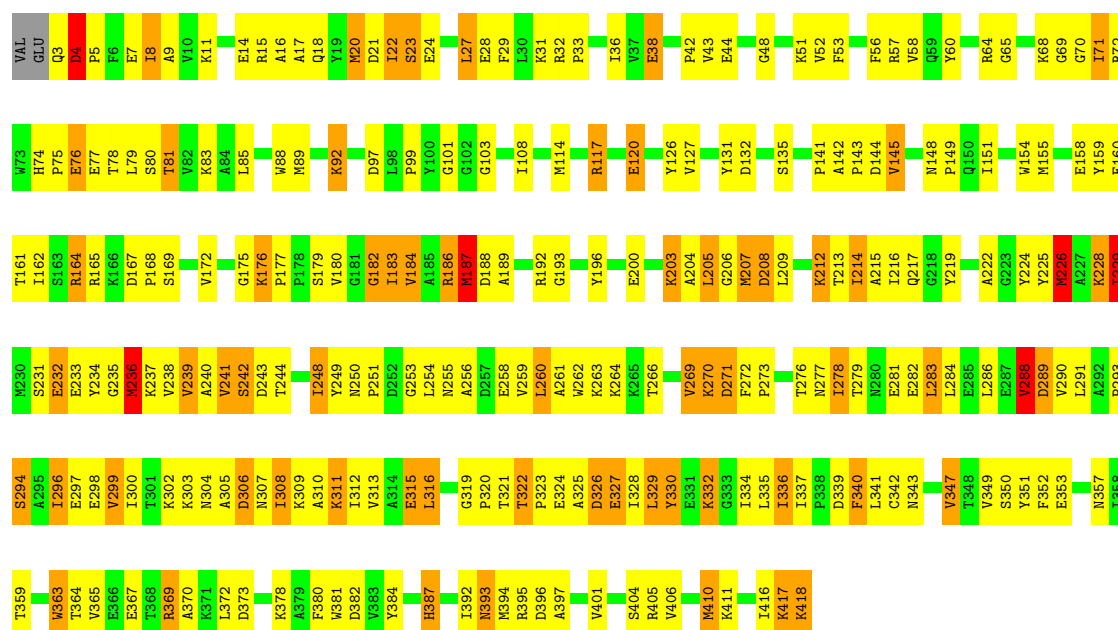
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)





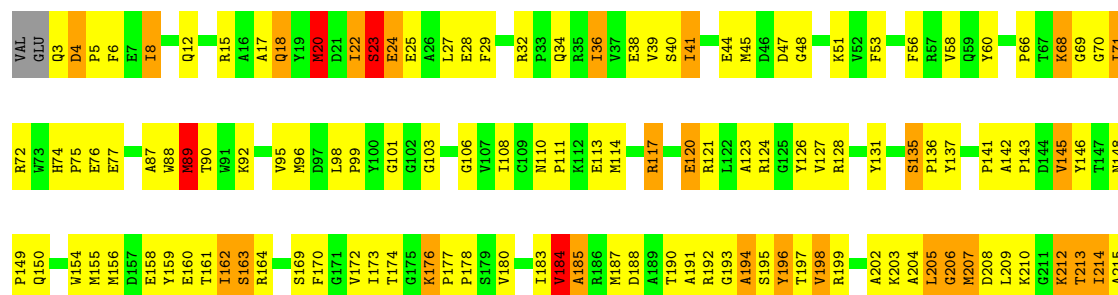
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

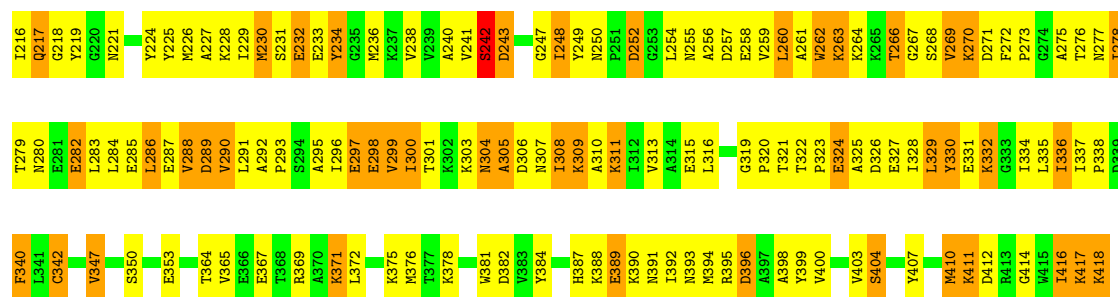
Chain C: 39% 44% 15% .



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

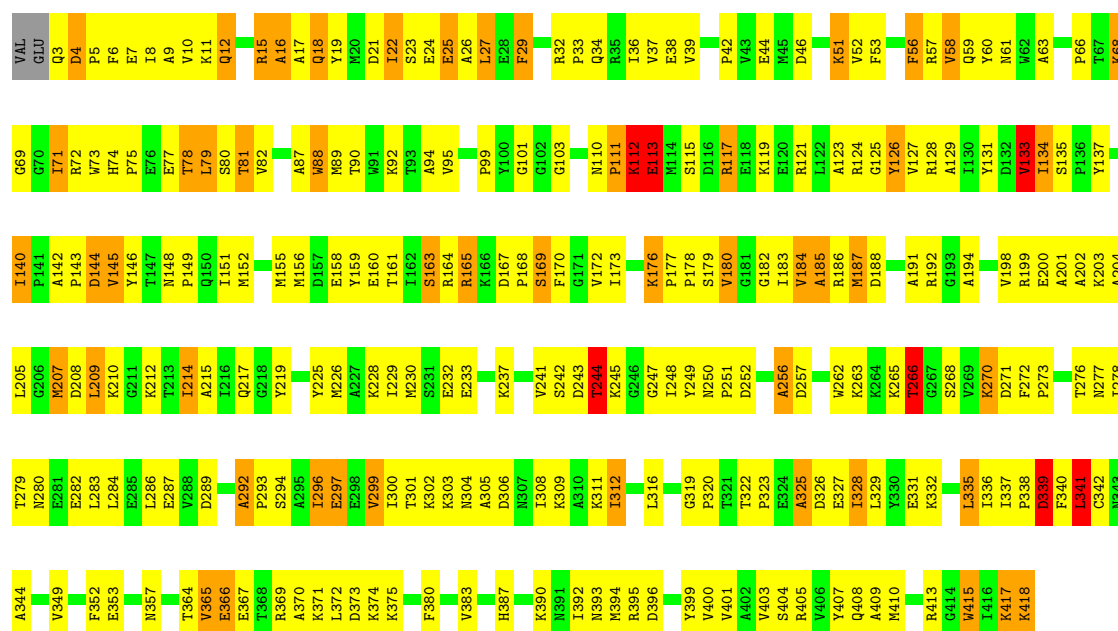
Chain D: 35% 46% 17% .





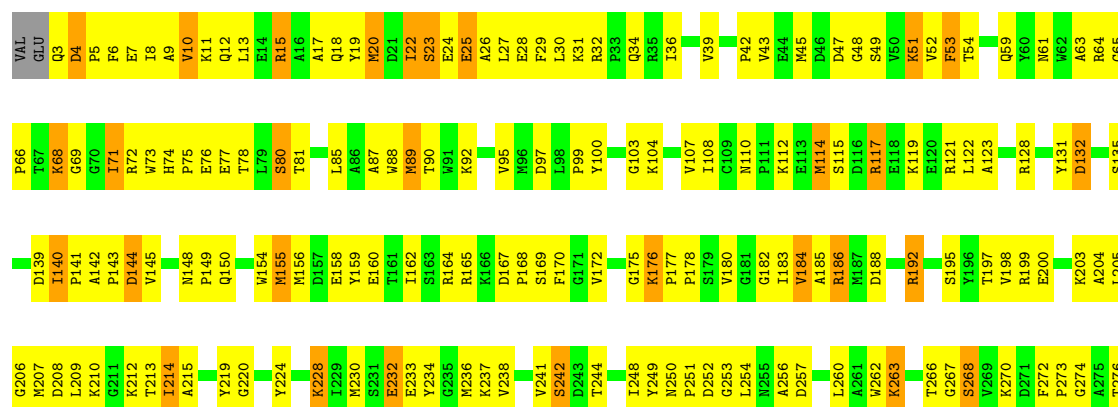
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain E: 37% 49% 12%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain F: 38% 48% 14%



N277	I278	T279	N280	E281	E282	L283	L284	E285	L286	E287	V288		L291	A292	P293	S294	A295	I296	E297	E298	V299	I300	T301	K302	K303	N304	A305	D306		K309	A310	K311	I312	V313		L316		G319	P320	T322	T321	P323	E324	A325	D326	E327	I328	L329		K332	G333	I334	L335	I336	I337	P338	D339	F340	L341
C342	N343	A344	G345	G346	V347	T348	V349	S350	Y351	F352	E353		W363	T364	V365	E366	E367	T368	R369		L372	D373	K374	K375		K378	A379		V383		H387	K388	E389	K390	N391	I392	N393	M394	R395	D396		Y399	V400	V401	A402	V403	S404		Y407		M410	K411		G414	W415	I416	K417	K418	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.90Å 197.50Å 125.70Å 90.00° 113.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	87.0 (10.00-2.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19566	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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	0.87	1/3331 (0.0%)	1.29	30/4511 (0.7%)
1	B	0.91	3/3331 (0.1%)	1.25	18/4511 (0.4%)
1	C	0.90	4/3331 (0.1%)	1.27	34/4511 (0.8%)
1	D	0.90	3/3331 (0.1%)	1.25	31/4511 (0.7%)
1	E	0.95	6/3331 (0.2%)	1.32	30/4511 (0.7%)
1	F	0.91	2/3331 (0.1%)	1.28	24/4511 (0.5%)
All	All	0.91	19/19986 (0.1%)	1.28	167/27066 (0.6%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	410	MET	SD-CE	-8.58	1.58	1.79
1	A	410	MET	SD-CE	-7.52	1.60	1.79
1	D	45	MET	SD-CE	-7.24	1.61	1.79
1	C	127	VAL	CA-CB	-6.52	1.47	1.54
1	F	156	MET	SD-CE	-6.19	1.64	1.79

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	GLU	N-CA-C	-9.95	100.42	111.07
1	E	299	VAL	N-CA-C	-9.36	104.36	113.53
1	A	325	ALA	N-CA-C	-9.12	101.34	111.28
1	A	241	VAL	N-CA-C	-8.79	98.10	108.82
1	B	341	LEU	N-CA-C	-8.73	101.32	112.93

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	3261	0	3254	336	0
1	B	3261	0	3254	257	0
1	C	3261	0	3254	283	0
1	D	3261	0	3254	322	0
1	E	3261	0	3254	272	0
1	F	3261	0	3254	259	0
All	All	19566	0	19524	1675	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 1675 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:A:329:LEU:HD23	1:A:334:ILE:CD1	1.54	1.36
1:D:255:ASN:O	1:D:259:VAL:HG23	1.25	1.30
1:A:279:THR:HG22	1:A:282:GLU:OE2	1.28	1.27
1:A:329:LEU:CD2	1:A:334:ILE:HD12	1.63	1.27
1:C:384:TYR:HD1	1:C:394:MET:CE	1.49	1.25

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	414/418 (99%)	355 (86%)	48 (12%)	11 (3%)	4 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	414/418 (99%)	370 (89%)	39 (9%)	5 (1%)	10	20
1	C	414/418 (99%)	355 (86%)	53 (13%)	6 (1%)	9	17
1	D	414/418 (99%)	356 (86%)	49 (12%)	9 (2%)	5	9
1	E	414/418 (99%)	366 (88%)	38 (9%)	10 (2%)	4	8
1	F	414/418 (99%)	359 (87%)	45 (11%)	10 (2%)	4	8
All	All	2484/2508 (99%)	2161 (87%)	272 (11%)	51 (2%)	5	9

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	B	4	ASP
1	C	4	ASP
1	D	4	ASP
1	D	305	ALA

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	342/344 (99%)	273 (80%)	69 (20%)	1	2
1	B	342/344 (99%)	284 (83%)	58 (17%)	2	4
1	C	342/344 (99%)	270 (79%)	72 (21%)	1	2
1	D	342/344 (99%)	269 (79%)	73 (21%)	1	2
1	E	342/344 (99%)	279 (82%)	63 (18%)	1	3
1	F	342/344 (99%)	280 (82%)	62 (18%)	2	3
All	All	2052/2064 (99%)	1655 (81%)	397 (19%)	1	2

5 of 397 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	231	SER

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Mol	Chain	Res	Type
1	E	71	ILE
1	D	282	GLU
1	D	369	ARG
1	E	163	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	110	ASN
1	F	3	GLN
1	E	150	GLN
1	E	385	ASN
1	F	217	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

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.