



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:48 AM UTC

PDB ID : 3AOE / pdb_00003aoe
Title : Crystal structure of hetero-hexameric glutamate dehydrogenase from *Thermus thermophilus* (Leu bound form)
Authors : Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on : 2010-09-27
Resolution : 2.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

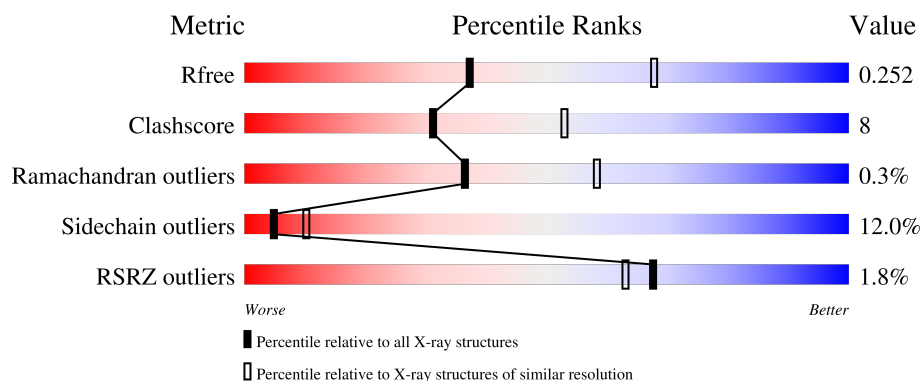
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	424	
1	B	424	
2	C	419	
2	D	419	
2	E	419	

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Mol	Chain	Length	Quality of chain
2	F	419	7% 78% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19355 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.

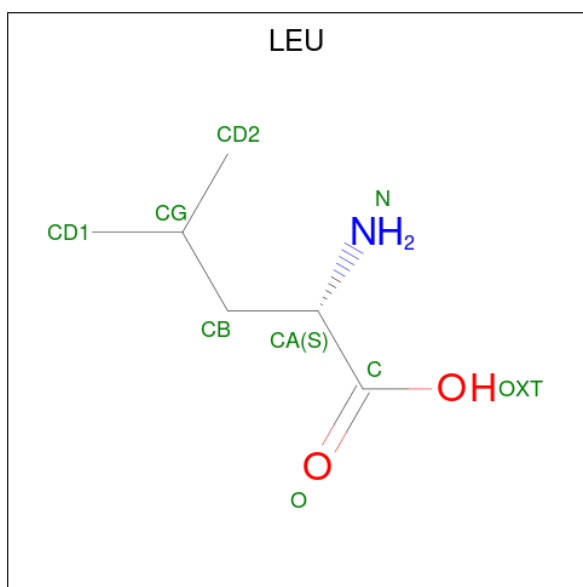
- Molecule 1 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	1	0
			3250	2068	583	593	6			
1	B	424	Total	C	N	O	S	0	1	0
			3267	2079	586	595	7			

- Molecule 2 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	416	Total	C	N	O	S	0	0	0
			3114	1972	552	579	11			
2	F	417	Total	C	N	O	S	0	0	0
			3122	1978	553	580	11			
2	C	417	Total	C	N	O	S	0	0	0
			3122	1978	553	580	11			
2	D	416	Total	C	N	O	S	0	0	0
			3114	1972	552	579	11			

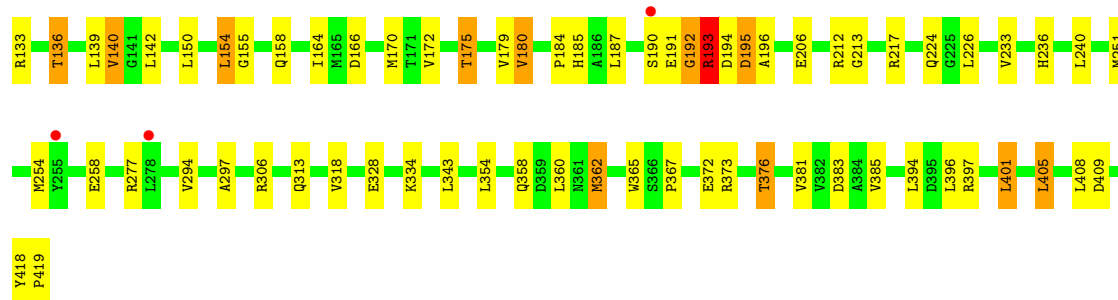
- Molecule 3 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂).



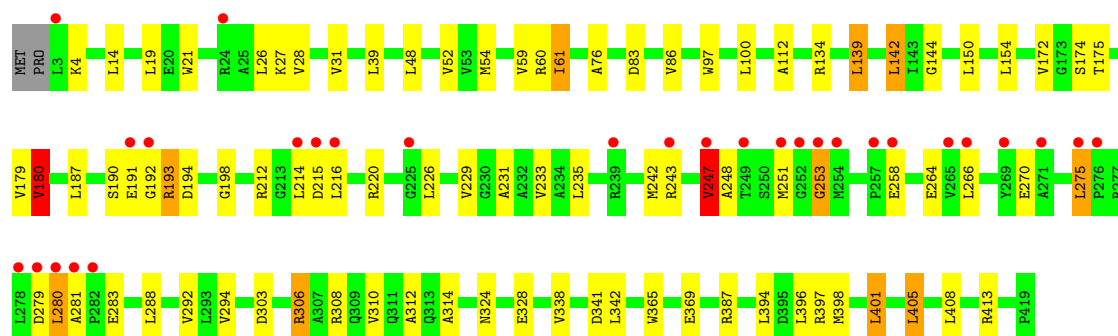
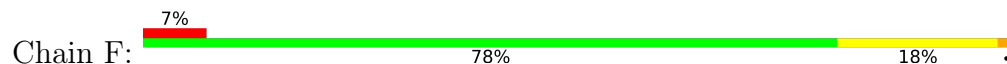
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	E	1	Total	C	N	O	0	0
			9	6	1	2		
3	F	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is water.

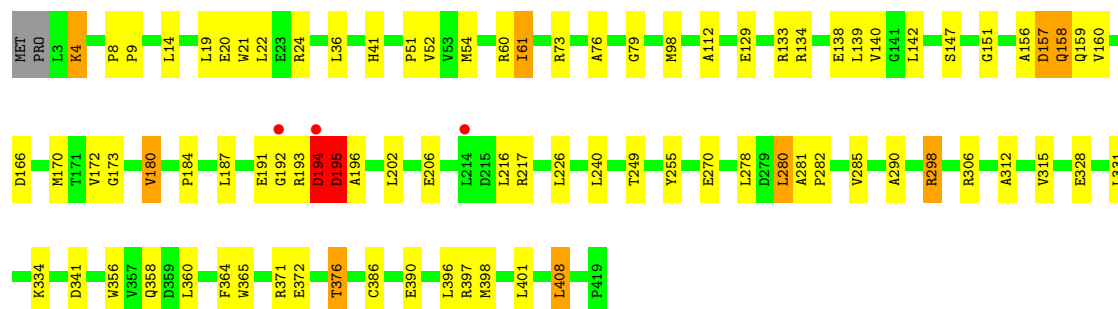
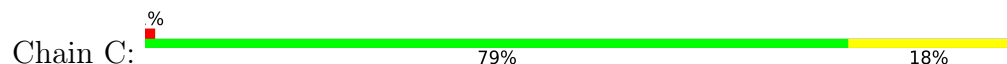
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	58	Total	O	0	0
			58	58		
4	E	55	Total	O	0	0
			55	55		
4	F	28	Total	O	0	0
			28	28		
4	C	57	Total	O	0	0
			57	57		
4	D	61	Total	O	0	0
			61	61		



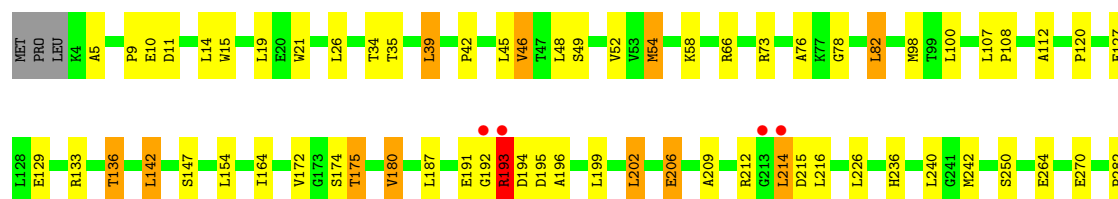
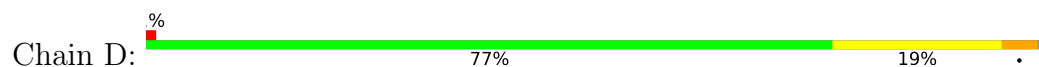
• Molecule 2: Glutamate dehydrogenase

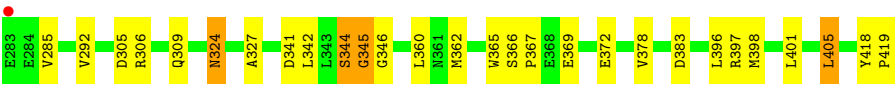


• Molecule 2: Glutamate dehydrogenase



• Molecule 2: Glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.99Å 146.09Å 158.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.22 – 2.60 30.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.22-2.60) 99.9 (30.22-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.193 , 0.260 0.188 , 0.252	Depositor DCC
R_{free} test set	4388 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19355	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.79	1/3330 (0.0%)	1.00	5/4532 (0.1%)
1	B	0.75	0/3347	0.97	3/4553 (0.1%)
2	C	0.75	0/3179	1.00	6/4320 (0.1%)
2	D	0.76	0/3171	1.05	8/4309 (0.2%)
2	E	0.74	1/3171 (0.0%)	0.99	6/4309 (0.1%)
2	F	0.73	0/3179	0.97	6/4320 (0.1%)
All	All	0.75	2/19377 (0.0%)	1.00	34/26343 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	11	ASP	CA-C	6.44	1.57	1.53
1	A	51	VAL	CA-CB	5.50	1.59	1.54

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	195	ASP	N-CA-C	-10.06	100.32	112.59
1	B	26	VAL	CA-C-N	7.12	124.73	120.24
1	B	26	VAL	C-N-CA	7.12	124.73	120.24
2	C	180	VAL	CB-CA-C	-6.76	98.60	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	LYS	N-CA-C	6.56	119.53	110.35

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	194	ASP	Peptide
2	D	345	GLY	Peptide
2	E	192	GLY	Peptide
2	F	193	ARG	Peptide

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	3250	0	3243	63	0
1	B	3267	0	3268	53	0
2	C	3122	0	3164	45	0
2	D	3114	0	3153	51	0
2	E	3114	0	3153	64	0
2	F	3122	0	3164	54	0
3	A	9	0	10	0	0
3	B	9	0	10	2	0
3	C	9	0	10	0	0
3	D	9	0	10	1	0
3	E	9	0	10	0	0
3	F	9	0	10	0	0
4	A	53	0	0	1	0
4	B	58	0	0	3	0
4	C	57	0	0	0	0
4	D	61	0	0	2	0
4	E	55	0	0	1	0
4	F	28	0	0	0	0
All	All	19355	0	19205	315	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 8.

The worst 5 of 315 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)
2:E:193:ARG:HB3	2:E:195:ASP:HB3	1.25	1.13
2:D:192:GLY:HA2	2:D:193:ARG:HB3	1.30	1.12
2:F:192:GLY:HA2	2:F:193:ARG:HB2	1.12	1.11
1:A:9:LEU:HD11	1:A:93:MET:HE1	1.31	1.10
2:C:298:ARG:HG2	2:C:298:ARG:HH11	1.21	1.02

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	421/424 (99%)	407 (97%)	13 (3%)	1 (0%)	43	66
1	B	423/424 (100%)	409 (97%)	14 (3%)	0	100	100
2	C	415/419 (99%)	400 (96%)	14 (3%)	1 (0%)	43	66
2	D	414/419 (99%)	399 (96%)	14 (3%)	1 (0%)	43	66
2	E	414/419 (99%)	392 (95%)	20 (5%)	2 (0%)	24	46
2	F	415/419 (99%)	375 (90%)	38 (9%)	2 (0%)	24	46
All	All	2502/2524 (99%)	2382 (95%)	113 (4%)	7 (0%)	36	58

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	193	ARG
2	F	253	GLY
2	F	247	VAL
2	C	192	GLY
2	D	193	ARG

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	327/328 (100%)	285 (87%)	42 (13%)	4	8
1	B	329/328 (100%)	297 (90%)	32 (10%)	8	17
2	C	312/314 (99%)	278 (89%)	34 (11%)	6	13
2	D	311/314 (99%)	268 (86%)	43 (14%)	3	7
2	E	311/314 (99%)	272 (88%)	39 (12%)	4	9
2	F	312/314 (99%)	275 (88%)	37 (12%)	5	10
All	All	1902/1912 (100%)	1675 (88%)	227 (12%)	5	10

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	26	LEU
2	D	372	GLU
2	F	338	VAL
2	D	342	LEU
2	D	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	228	GLN
2	D	309	GLN
2	D	361	ASN
1	B	310	GLN
1	B	306	GLN

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LEU	A	500	-	6,8,8	1.15	1 (16%)	5,10,10	1.39	1 (20%)
3	LEU	B	500	-	6,8,8	0.92	1 (16%)	5,10,10	1.63	1 (20%)
3	LEU	E	500	-	6,8,8	0.85	0	5,10,10	1.22	1 (20%)
3	LEU	C	500	-	6,8,8	0.82	0	5,10,10	0.90	0
3	LEU	D	500	-	6,8,8	1.01	1 (16%)	5,10,10	1.32	1 (20%)
3	LEU	F	500	-	6,8,8	0.88	0	5,10,10	1.20	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LEU	A	500	-	-	1/8/8/8	-
3	LEU	B	500	-	-	0/8/8/8	-
3	LEU	E	500	-	-	5/8/8/8	-
3	LEU	C	500	-	-	0/8/8/8	-
3	LEU	D	500	-	-	4/8/8/8	-
3	LEU	F	500	-	-	0/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	LEU	OXT-C	-2.56	1.22	1.30
3	D	500	LEU	OXT-C	-2.26	1.23	1.30
3	B	500	LEU	OXT-C	-2.08	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	LEU	OXT-C-O	-3.31	116.56	124.08
3	A	500	LEU	OXT-C-O	-2.87	117.57	124.08
3	E	500	LEU	OXT-C-O	-2.45	118.53	124.08
3	D	500	LEU	OXT-C-O	-2.36	118.73	124.08
3	F	500	LEU	OXT-C-O	-2.25	118.97	124.08

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	500	LEU	N-CA-CB-CG
3	E	500	LEU	C-CA-CB-CG
3	E	500	LEU	CA-CB-CG-CD1
3	E	500	LEU	CA-CB-CG-CD2
3	D	500	LEU	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	LEU	2	0
3	D	500	LEU	1	0

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/424 (99%)	-0.48	2 (0%) 87 85	17, 38, 57, 71	2 (0%)
1	B	424/424 (100%)	-0.40	3 (0%) 84 82	16, 39, 70, 85	1 (0%)
2	C	417/419 (99%)	-0.40	3 (0%) 84 82	25, 39, 61, 75	0
2	D	416/419 (99%)	-0.40	5 (1%) 76 73	25, 40, 62, 75	0
2	E	416/419 (99%)	-0.28	4 (0%) 79 76	25, 43, 76, 83	1 (0%)
2	F	417/419 (99%)	0.04	29 (6%) 22 18	26, 45, 117, 125	1 (0%)
All	All	2512/2524 (99%)	-0.32	46 (1%) 67 63	16, 40, 77, 125	5 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	192	GLY	5.2
2	F	192	GLY	4.1
1	B	13	GLY	3.9
2	F	278	LEU	3.9
2	C	214	LEU	3.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LEU	B	500	9/9	0.93	0.09	40,40,41,43	0
3	LEU	D	500	9/9	0.94	0.09	25,29,29,30	0
3	LEU	F	500	9/9	0.95	0.07	33,33,34,36	0
3	LEU	A	500	9/9	0.96	0.06	28,31,31,34	0
3	LEU	E	500	9/9	0.96	0.07	29,30,30,31	0
3	LEU	C	500	9/9	0.97	0.06	31,33,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.