WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2024 – 04:53 PM EDT

PDB ID	:	3AOE
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)

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.252
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		11.8%
RSRZ outliers		3.0%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
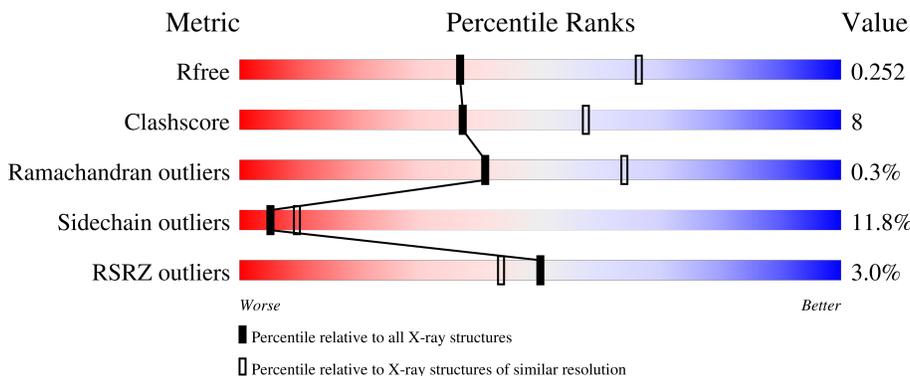
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	% 76% 19% •
1	B	424	3% 80% 17% •
2	C	419	% 80% 17% •
2	D	419	2% 78% 18% ••
2	E	419	2% 77% 19% ••

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Mol	Chain	Length	Quality of chain
2	F	419	9% ... 80% ... 17% ...

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 3250	C 2068	N 583	O 593	S 6	0	1	0
1	B	424	Total 3267	C 2079	N 586	O 595	S 7	0	1	0

- Molecule 2 is a protein called Glutamate dehydrogenase.

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

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).
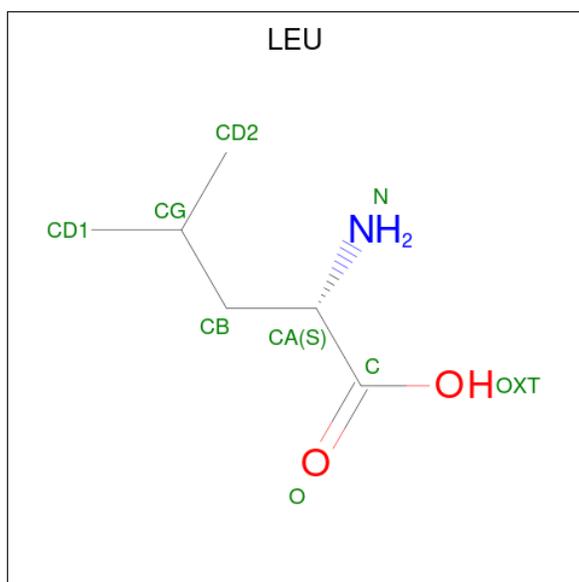
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 6	N 1	O 2	0	0
3	B	1	Total 9	C 6	N 1	O 2	0	0
3	E	1	Total 9	C 6	N 1	O 2	0	0
3	F	1	Total 9	C 6	N 1	O 2	0	0
3	C	1	Total 9	C 6	N 1	O 2	0	0
3	D	1	Total 9	C 6	N 1	O 2	0	0

- Molecule 4 is water.

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

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 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.

- Molecule 1: Glutamate dehydrogenase

Chain A:

- Molecule 1: Glutamate dehydrogenase

Chain B:

- Molecule 2: Glutamate dehydrogenase

Chain E:

L142 L150 L154 G155 Q158 I164 M165 D166 M170 T171 V172 T175 V179 V180 P184 H185 A186 L187 S190 E191 G192 R193 D194 D195 A196 E206 R212 G213 L214 D215 L216 R217 Q224 V233 H236 L240 M251 E258 E264 G273 S274

L275 L278 P282 V294 A297 D305 R306 A307 R308 Q313 E328 K334 L343 L354 Q358 D359 L360 N361 M362 W365 S366 P367 E372 R373 T376 D383 A384 V385 R391 L394 D395 L396 R397 L401 L405 L408 D409 Y418 P419

• Molecule 2: Glutamate dehydrogenase

Chain F:

MET PRO L3 L14 L19 L26 K27 G30 V31 L39 L48 V52 V53 M54 V59 R60 I61 A76 D83 V86 W97 L100 A112 L123 R134 L139 L142 I143 G144 L150 L154 V172 G173 S174 T175 V179 V180

L187 S190 E191 G192 R193 G198 R211 R212 G213 L214 D215 I216 R217 R220 L226 V229 G230 A231 A232 V233 A234 L235 R243 V247 A248 M251 G252 G253 M254 Y255 A256 P257 E258 A263 E264 V265 L266 S267 A268 Y269 E270 A271 T272 L275 P276 R277 L278 D279 L280

A281 P282 E283 L288 E289 A290 E291 V292 L293 V294 D303 G304 D305 R306 A307 R308 Q309 V310 Q311 A312 Q313 A314 N324 E326 A327 E328 A329 Y330 G335 D341 L342 W365 E369 R387 R391 L394 D395 L396 M398 L401 L405 L408 R413

P419

• Molecule 2: Glutamate dehydrogenase

Chain C:

MET PRO L3 K4 P8 P9 L14 L19 E20 W21 L22 L26 K27 L36 H41 P51 V52 V53 M54 R60 I61 R73 A76 G79 W97 A112 Q126 E129 R133 R134 E138 L139 L142 S147 G151 D157 Q158 Q159 V160

D166 M170 T171 V172 G173 V180 P184 L187 E191 G192 R193 D194 D195 A196 L202 E206 G213 L214 D215 L216 R217 L226 T249 Y255 E270 L278 D279 L280 A281 P282 V285 A290 R298 D305 R306 A312 V315 E328

L331 K334 D341 W356 V357 Q358 D359 L360 W365 R371 E372 T376 C386 E390 L396 R397 L401 L408 P419

• Molecule 2: Glutamate dehydrogenase

Chain D:

MET PRO LEU K4 R7 P8 P9 E10 D11 L14 W15 L19 E20 W21 L26 T34 T35 L39 P42 L45 V46 T47 L48 S49 V52 V53 M54 K58 R66 R73 A76 L82 W97 M98 T99 L100 L107 P108 A112 P120 E127

L128 E129 R133 T136 L142 S147 L154 I164 S174 T175 V180 L187 E191 G192 R193 D194 D195 A196 L199 L202 E206 A209 R212 G213 L214 D215 L216 R217 L226 H236 L240 G241 M242 M251 E264 S267 E270

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) 100.0 (30.22-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.36 , 36.4	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.65	0/3330	0.73	2/4532 (0.0%)
1	B	0.62	0/3347	0.72	2/4553 (0.0%)
2	C	0.62	0/3179	0.77	3/4320 (0.1%)
2	D	0.62	0/3171	0.77	3/4309 (0.1%)
2	E	0.58	0/3171	0.71	0/4309
2	F	0.58	0/3179	0.71	2/4320 (0.0%)
All	All	0.61	0/19377	0.73	12/26343 (0.0%)

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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	402	ARG	NE-CZ-NH2	6.89	123.74	120.30
2	C	180	VAL	CB-CA-C	-6.74	98.60	111.40
1	A	74	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	402	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	D	48	LEU	CA-CB-CG	5.90	128.88	115.30

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	59	0
1	B	3267	0	3268	52	0
2	C	3122	0	3164	44	0
2	D	3114	0	3153	44	0
2	E	3114	0	3153	63	0
2	F	3122	0	3164	50	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	297	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 297 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD11	1:A:93:MET:HE1	1.32	1.11
2:F:192:GLY:HA2	2:F:193:ARG:HB2	1.12	1.11
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%)	47	71
1	B	423/424 (100%)	409 (97%)	14 (3%)	0	100	100
2	C	415/419 (99%)	400 (96%)	14 (3%)	1 (0%)	47	71
2	D	414/419 (99%)	399 (96%)	14 (3%)	1 (0%)	47	71
2	E	414/419 (99%)	392 (95%)	20 (5%)	2 (0%)	29	52
2	F	415/419 (99%)	375 (90%)	38 (9%)	2 (0%)	29	52
All	All	2502/2524 (99%)	2382 (95%)	113 (4%)	7 (0%)	41	64

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%)	289 (88%)	38 (12%)	5	10
1	B	329/328 (100%)	298 (91%)	31 (9%)	8	17
2	C	312/314 (99%)	278 (89%)	34 (11%)	6	11
2	D	311/314 (99%)	267 (86%)	44 (14%)	3	6
2	E	311/314 (99%)	273 (88%)	38 (12%)	5	9
2	F	312/314 (99%)	275 (88%)	37 (12%)	5	9
All	All	1902/1912 (100%)	1680 (88%)	222 (12%)	5	10

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	142	LEU
2	D	401	LEU
2	F	413	ARG
2	D	396	LEU
2	D	187	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	C	358	GLN
2	D	159	GLN
2	D	324	ASN
1	B	306	GLN
1	B	225	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 monosaccharides 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	E	500	-	7,8,8	0.80	0	9,10,10	1.22	2 (22%)
3	LEU	A	500	-	7,8,8	1.03	1 (14%)	9,10,10	1.21	1 (11%)
3	LEU	B	500	-	7,8,8	0.82	0	9,10,10	1.43	2 (22%)
3	LEU	F	500	-	7,8,8	0.83	0	9,10,10	1.09	1 (11%)
3	LEU	D	500	-	7,8,8	0.90	1 (14%)	9,10,10	1.28	2 (22%)
3	LEU	C	500	-	7,8,8	0.73	0	9,10,10	1.07	1 (11%)

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	E	500	-	-	5/8/8/8	-
3	LEU	A	500	-	-	1/8/8/8	-
3	LEU	B	500	-	-	0/8/8/8	-
3	LEU	F	500	-	-	0/8/8/8	-
3	LEU	D	500	-	-	3/8/8/8	-
3	LEU	C	500	-	-	0/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	LEU	OXT-C	-2.47	1.22	1.30
3	D	500	LEU	OXT-C	-2.16	1.23	1.30

The worst 5 of 9 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	124.09
3	A	500	LEU	OXT-C-O	-2.87	117.57	124.09
3	E	500	LEU	OXT-C-O	-2.45	118.53	124.09
3	D	500	LEU	OXT-C-O	-2.36	118.73	124.09
3	D	500	LEU	OXT-C-CA	2.32	121.30	113.38

There are no chirality outliers.

5 of 9 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 ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	422/424 (99%)	-0.43	5 (1%)	79	76	24, 38, 57, 71	1 (0%)
1	B	424/424 (100%)	-0.37	11 (2%)	56	50	25, 39, 70, 85	0
2	C	417/419 (99%)	-0.33	6 (1%)	75	71	25, 39, 61, 75	0
2	D	416/419 (99%)	-0.29	7 (1%)	70	66	25, 40, 62, 75	0
2	E	416/419 (99%)	-0.20	10 (2%)	59	53	25, 43, 76, 83	1 (0%)
2	F	417/419 (99%)	0.05	37 (8%)	9	6	26, 45, 117, 125	1 (0%)
All	All	2512/2524 (99%)	-0.26	76 (3%)	50	43	24, 40, 77, 125	3 (0%)

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	252	GLY	5.4
2	D	213	GLY	4.9
2	F	280	LEU	4.8
2	D	192	GLY	4.8
2	F	257	PRO	4.4

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	0.95	0.16	40,40,41,43	0
3	LEU	F	500	9/9	0.96	0.17	33,33,34,36	0
3	LEU	D	500	9/9	0.96	0.18	25,29,29,30	0
3	LEU	A	500	9/9	0.97	0.13	28,31,31,34	0
3	LEU	C	500	9/9	0.98	0.18	31,33,33,34	0
3	LEU	E	500	9/9	0.98	0.17	29,30,30,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.