



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:51 PM UTC

PDB ID : 4CTI / pdb_00004cti
Title : Escherichia coli EnvZ histidine kinase catalytic part fused to Archaeoglobus fulgidus Af1503 HAMP domain
Authors : Ferris, H.U.; Coles, M.; Lupas, A.N.; Hartmann, M.D.
Deposited on : 2014-03-13
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	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

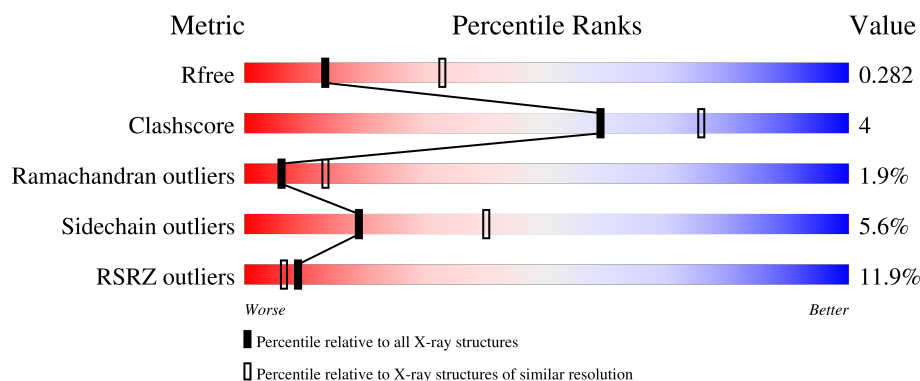
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	273	7% 65% 10% 24%
1	B	273	7% 69% 11% 19%
1	C	273	12% 63% 10% 26%
1	D	273	10% 65% 15% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6389 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 OSMOLARITY SENSOR PROTEIN ENVZ, AF1503.

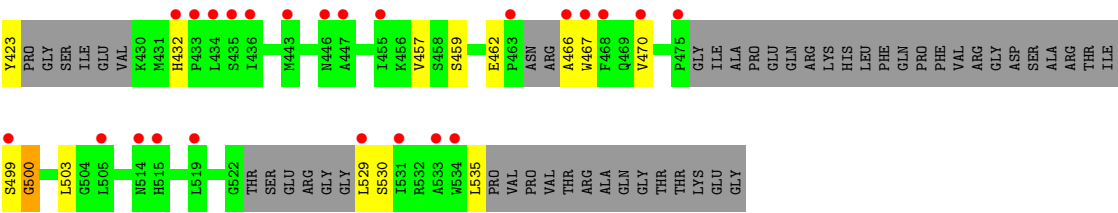
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1558	979	271	301	7			
1	B	222	Total	C	N	O	S	0	0	0
			1671	1050	288	325	8			
1	C	203	Total	C	N	O	S	0	0	0
			1508	943	264	294	7			
1	D	223	Total	C	N	O	S	0	0	0
			1652	1041	284	319	8			

There are 8 discrepancies between the modelled and reference sequences:

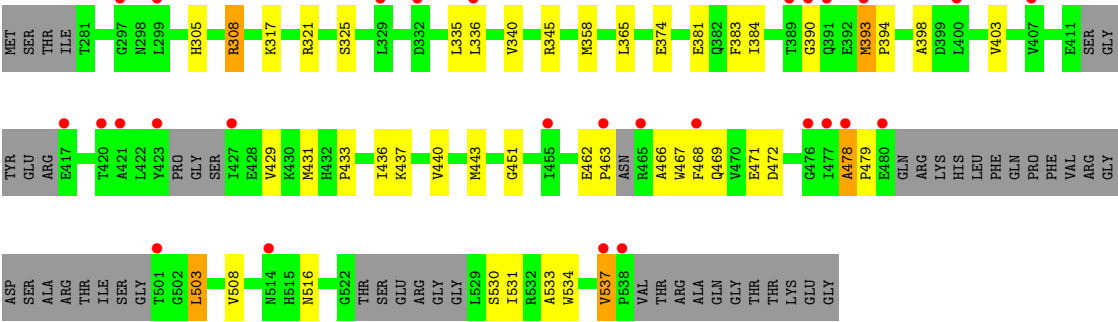
Chain	Residue	Modelled	Actual	Comment	Reference
A	277	MET	-	expression tag	UNP O28769
A	291	PHE	ALA	engineered mutation	UNP O28769
B	277	MET	-	expression tag	UNP O28769
B	291	PHE	ALA	engineered mutation	UNP O28769
C	277	MET	-	expression tag	UNP O28769
C	291	PHE	ALA	engineered mutation	UNP O28769
D	277	MET	-	expression tag	UNP O28769
D	291	PHE	ALA	engineered mutation	UNP O28769

- Molecule 1: OSMOLARITY SENSOR PROTEIN ENVZ, AF1503





● Molecule 1: OSMOLARITY SENSOR PROTEIN ENVZ, AF1503



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.06Å 76.62Å 97.37Å 90.00° 107.03° 90.00°	Depositor
Resolution (Å)	38.83 – 2.85 38.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.83-2.85) 99.3 (38.83-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.258 , 0.277 0.267 , 0.282	Depositor DCC
R_{free} test set	1170 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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	0.28	0/1574	0.73	2/2130 (0.1%)
1	B	0.29	0/1692	0.75	2/2296 (0.1%)
1	C	0.27	0/1519	0.74	2/2053 (0.1%)
1	D	0.29	0/1672	0.79	2/2270 (0.1%)
All	All	0.28	0/6457	0.75	8/8749 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	MET	CA-C-N	6.92	128.49	119.84
1	D	393	MET	C-N-CA	6.92	128.49	119.84
1	A	432	HIS	CA-C-N	5.88	125.36	119.24
1	A	432	HIS	C-N-CA	5.88	125.36	119.24
1	B	432	HIS	CA-C-N	5.38	124.83	119.24
1	B	432	HIS	C-N-CA	5.38	124.83	119.24
1	C	432	HIS	CA-C-N	5.16	124.61	119.24
1	C	432	HIS	C-N-CA	5.16	124.61	119.24

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	1558	0	1528	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1671	0	1631	15	0
1	C	1508	0	1485	12	0
1	D	1652	0	1608	22	0
All	All	6389	0	6252	56	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 4.

All (56) 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:382:GLN:NE2	1:A:500:GLY:O	2.23	0.71
1:D:429:VAL:HG12	1:D:537:VAL:HG22	1.72	0.70
1:D:469:GLN:HE21	1:D:530:SER:HB2	1.60	0.66
1:C:382:GLN:NE2	1:C:500:GLY:O	2.28	0.64
1:B:398:ALA:HB3	1:B:431:MET:HE2	1.82	0.60
1:B:462:GLU:HG3	1:B:463:PRO:HD2	1.84	0.59
1:C:457:VAL:HG22	1:C:470:VAL:HG22	1.85	0.58
1:D:451:GLY:HA3	1:D:472:ASP:HB2	1.86	0.57
1:B:403:VAL:HG21	1:B:431:MET:HE1	1.86	0.56
1:B:308:ARG:NH2	1:B:310:ASP:OD2	2.40	0.55
1:C:300:GLU:OE2	1:C:327:LYS:NZ	2.38	0.54
1:A:423:TYR:CD1	1:A:460:GLY:HA2	2.44	0.53
1:B:305:HIS:HB3	1:B:308:ARG:HD3	1.92	0.51
1:A:467:TRP:HA	1:A:533:ALA:O	2.11	0.51
1:D:469:GLN:NE2	1:D:471:GLU:OE2	2.44	0.51
1:C:325:SER:OG	1:D:516:ASN:OD1	2.23	0.51
1:D:305:HIS:HB3	1:D:308:ARG:HD3	1.93	0.51
1:C:405:GLY:HA2	1:C:408:ILE:HD12	1.91	0.50
1:D:443:MET:HE3	1:D:531:ILE:HB	1.92	0.50
1:A:405:GLY:HA2	1:A:408:ILE:HD12	1.92	0.50
1:D:443:MET:HG3	1:D:508:VAL:HG21	1.94	0.50
1:C:358:MET:HE3	1:D:358:MET:HE3	1.94	0.49
1:C:466:ALA:HB3	1:C:535:LEU:HB2	1.94	0.49
1:D:462:GLU:HG3	1:D:463:PRO:HD2	1.94	0.49
1:B:389:THR:OG1	1:B:438:ARG:NH1	2.46	0.48
1:C:423:TYR:H	1:C:459:SER:HB2	1.78	0.48
1:D:467:TRP:HA	1:D:533:ALA:O	2.14	0.48
1:D:403:VAL:HG21	1:D:431:MET:HE1	1.95	0.47
1:D:345:ARG:HH21	1:D:384:ILE:HD11	1.80	0.47
1:B:435:SER:HB3	1:B:511:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HB	1:A:312:ILE:HD11	1.98	0.45
1:C:383:PHE:CG	1:D:340:VAL:HG21	2.51	0.45
1:B:308:ARG:HE	1:B:308:ARG:HB3	1.56	0.44
1:D:398:ALA:HB3	1:D:431:MET:HE2	1.98	0.44
1:D:478:ALA:HA	1:D:479:PRO:HD3	1.88	0.44
1:A:435:SER:HB3	1:A:511:ILE:HG23	2.01	0.43
1:A:403:VAL:O	1:A:407:VAL:HG23	2.19	0.42
1:C:403:VAL:O	1:C:407:VAL:HG23	2.19	0.42
1:B:431:MET:SD	1:B:436:ILE:HG13	2.59	0.42
1:C:315:LEU:O	1:C:319:ILE:HG13	2.19	0.41
1:A:315:LEU:O	1:A:319:ILE:HG13	2.20	0.41
1:A:435:SER:O	1:A:511:ILE:HD13	2.20	0.41
1:B:386:TYR:OH	1:B:510:ARG:HG2	2.19	0.41
1:A:358:MET:HE3	1:B:358:MET:HE3	2.02	0.41
1:B:317:LYS:HB3	1:B:317:LYS:HE2	1.76	0.41
1:B:429:VAL:HG12	1:B:537:VAL:HG22	2.03	0.41
1:D:433:PRO:O	1:D:437:LYS:HB2	2.21	0.41
1:A:454:TRP:CD1	1:A:473:ASP:HB2	2.55	0.40
1:B:440:VAL:HG22	1:B:468:PHE:CE1	2.56	0.40
1:D:440:VAL:HG22	1:D:468:PHE:CZ	2.57	0.40
1:B:478:ALA:HA	1:B:479:PRO:HD3	1.96	0.40
1:D:383:PHE:HB2	1:D:503:LEU:HD11	2.02	0.40
1:D:466:ALA:O	1:D:534:TRP:HA	2.21	0.40
1:D:317:LYS:HB3	1:D:317:LYS:HE2	1.76	0.40
1:D:431:MET:SD	1:D:436:ILE:HG13	2.62	0.40
1:C:499:SER:OG	1:C:500:GLY:N	2.54	0.40

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	193/273 (71%)	185 (96%)	4 (2%)	4 (2%)	5	12
1	B	210/273 (77%)	197 (94%)	10 (5%)	3 (1%)	9	18
1	C	189/273 (69%)	182 (96%)	4 (2%)	3 (2%)	7	16
1	D	211/273 (77%)	196 (93%)	10 (5%)	5 (2%)	4	10
All	All	803/1092 (74%)	760 (95%)	28 (4%)	15 (2%)	6	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	394	PRO
1	A	467	TRP
1	C	467	TRP
1	A	462	GLU
1	C	462	GLU
1	A	453	GLY
1	B	480	GLU
1	B	537	VAL
1	D	478	ALA
1	D	537	VAL
1	B	478	ALA
1	D	393	MET
1	A	500	GLY
1	C	500	GLY
1	D	390	GLY

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	161/226 (71%)	152 (94%)	9 (6%)	19	40
1	B	173/226 (76%)	162 (94%)	11 (6%)	16	33
1	C	156/226 (69%)	148 (95%)	8 (5%)	21	44
1	D	168/226 (74%)	159 (95%)	9 (5%)	20	42
All	All	658/904 (73%)	621 (94%)	37 (6%)	19	40

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	LYS
1	A	334	THR
1	A	335	LEU
1	A	336	LEU
1	A	368	SER
1	A	467	TRP
1	A	503	LEU
1	A	529	LEU
1	A	530	SER
1	B	308	ARG
1	B	321	ARG
1	B	325	SER
1	B	335	LEU
1	B	336	LEU
1	B	365	LEU
1	B	374	GLU
1	B	423	TYR
1	B	428	GLU
1	B	432	HIS
1	B	503	LEU
1	C	327	LYS
1	C	334	THR
1	C	335	LEU
1	C	336	LEU
1	C	368	SER
1	C	503	LEU
1	C	529	LEU
1	C	530	SER
1	D	308	ARG
1	D	321	ARG
1	D	325	SER
1	D	335	LEU
1	D	336	LEU
1	D	365	LEU
1	D	374	GLU
1	D	381	GLU
1	D	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	C	306	GLN
1	C	509	GLN
1	D	432	HIS
1	D	469	GLN
1	D	509	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

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	207/273 (75%)	0.74	20 (9%)	13 10	53, 91, 169, 202	0
1	B	222/273 (81%)	0.80	20 (9%)	15 12	55, 91, 163, 189	0
1	C	203/273 (74%)	1.03	34 (16%)	4 3	64, 104, 306, 412	0
1	D	223/273 (81%)	0.85	28 (12%)	8 5	60, 98, 167, 206	0
All	All	855/1092 (78%)	0.85	102 (11%)	9 6	53, 95, 251, 412	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	514	ASN	5.3
1	C	519	LEU	4.8
1	B	329	LEU	4.6
1	D	468	PHE	4.6
1	C	468	PHE	4.3
1	C	531	ILE	4.3
1	B	538	PRO	4.2
1	C	447	ALA	4.0
1	D	538	PRO	3.9
1	C	446	ASN	3.9
1	A	331	ASP	3.8
1	D	477	ILE	3.7
1	B	390	GLY	3.6
1	D	501	THR	3.5
1	D	299	LEU	3.5
1	C	499	SER	3.4
1	D	480	GLU	3.3
1	A	407	VAL	3.3
1	A	519	LEU	3.3
1	B	336	LEU	3.3
1	C	470	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	307	ASN	3.3
1	A	444	VAL	3.2
1	C	467	TRP	3.2
1	D	297	GLY	3.2
1	C	409	ALA	3.2
1	B	407	VAL	3.2
1	D	476	GLY	3.2
1	A	499	SER	3.1
1	D	332	ASP	3.1
1	B	481	GLN	3.0
1	C	407	VAL	3.0
1	D	420	THR	3.0
1	D	391	GLN	3.0
1	C	505	LEU	2.9
1	D	463	PRO	2.9
1	A	529	LEU	2.8
1	A	463	PRO	2.8
1	C	466	ALA	2.8
1	C	533	ALA	2.7
1	C	332	ASP	2.7
1	A	440	VAL	2.7
1	C	515	HIS	2.7
1	D	336	LEU	2.7
1	D	421	ALA	2.7
1	C	404	LEU	2.7
1	D	465	ARG	2.7
1	C	434	LEU	2.7
1	C	534	TRP	2.6
1	C	529	LEU	2.6
1	B	478	ALA	2.6
1	B	394	PRO	2.6
1	D	455	ILE	2.6
1	C	309	ALA	2.5
1	B	466	ALA	2.5
1	D	478	ALA	2.5
1	B	479	PRO	2.5
1	A	431	MET	2.5
1	A	521	LEU	2.5
1	B	518	MET	2.5
1	D	329	LEU	2.5
1	C	463	PRO	2.5
1	B	477	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	389	THR	2.5
1	C	443	MET	2.4
1	D	417	GLU	2.4
1	C	435	SER	2.4
1	C	433	PRO	2.4
1	C	432	HIS	2.4
1	C	408	ILE	2.4
1	C	403	VAL	2.4
1	A	332	ASP	2.4
1	D	407	VAL	2.3
1	D	400	LEU	2.3
1	C	436	ILE	2.3
1	B	423	TYR	2.3
1	D	423	TYR	2.3
1	C	406	GLU	2.3
1	C	417	GLU	2.3
1	D	514	ASN	2.2
1	A	472	ASP	2.2
1	B	465	ARG	2.2
1	A	406	GLU	2.2
1	A	408	ILE	2.2
1	C	475	PRO	2.2
1	D	393	MET	2.2
1	D	427	ILE	2.2
1	A	409	ALA	2.2
1	B	400	LEU	2.1
1	A	462	GLU	2.1
1	B	411	GLU	2.1
1	D	537	VAL	2.1
1	A	423	TYR	2.1
1	A	447	ALA	2.1
1	B	476	GLY	2.1
1	B	372	ASP	2.1
1	B	501	THR	2.1
1	C	455	ILE	2.1
1	D	390	GLY	2.0
1	A	342	HIS	2.0
1	B	418	ILE	2.0
1	C	312	ILE	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.