Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2025 – 04:05 PM EDT

PDB ID : 9EIR
Title : Ethylene-forming enzyme apoprotein from Penicillium digitatum
Authors : Chatterjee, S.; Rankin, J.A.; Farrugia, M.A.; Hu, J.; Hausinger, R.P.
Deposited on : 2024-11-26
Resolution : 3.50 Å(reported)

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

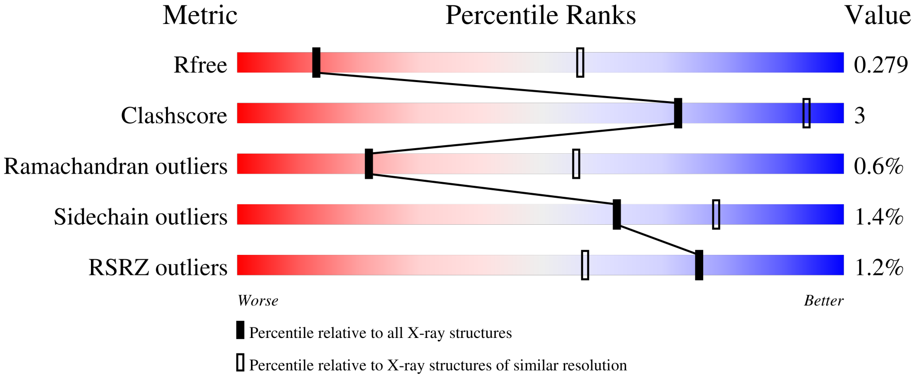
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

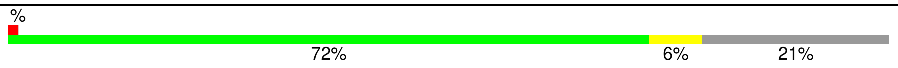
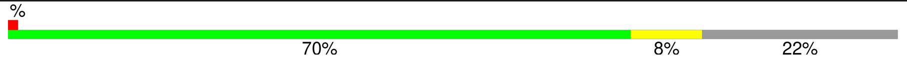
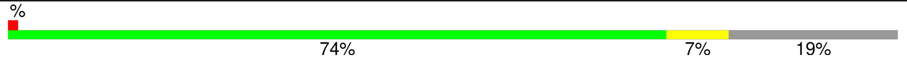
The reported resolution of this entry is 3.50 Å.

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))
R_{free}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	407	
1	B	407	
1	C	407	
1	D	407	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9361 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 2-oxoglutarate-dependent ethylene/succinate-forming enzyme.

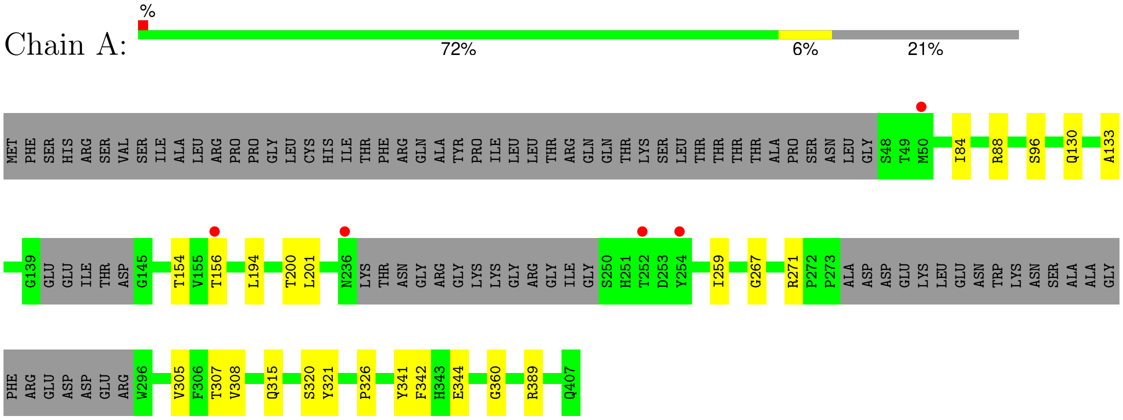
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total 2316	C 1499	N 399	O 405	S 13	0	0	0
1	B	312	Total 2263	C 1475	N 382	O 393	S 13	0	0	0
1	C	319	Total 2370	C 1528	N 399	O 429	S 14	0	0	0
1	D	329	Total 2412	C 1563	N 411	O 425	S 13	0	0	0

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.

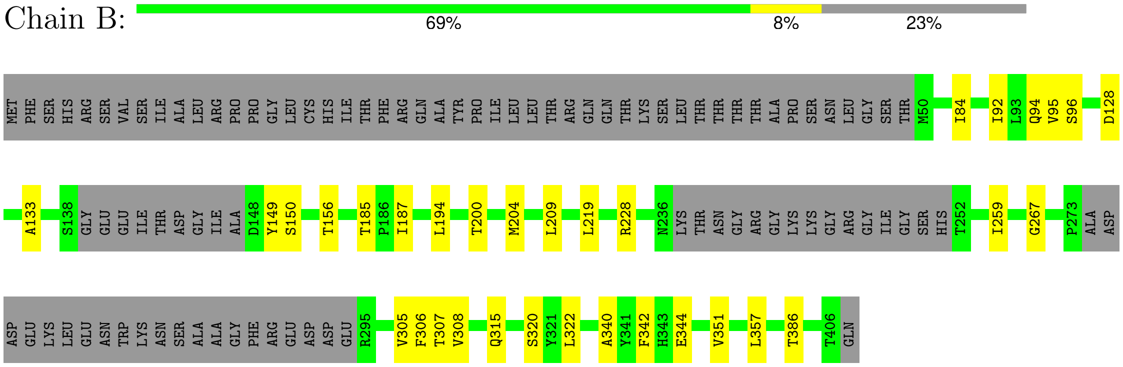
- Molecule 1: 2-oxoglutarate-dependent ethylene/succinate-forming enzyme

Chain A:



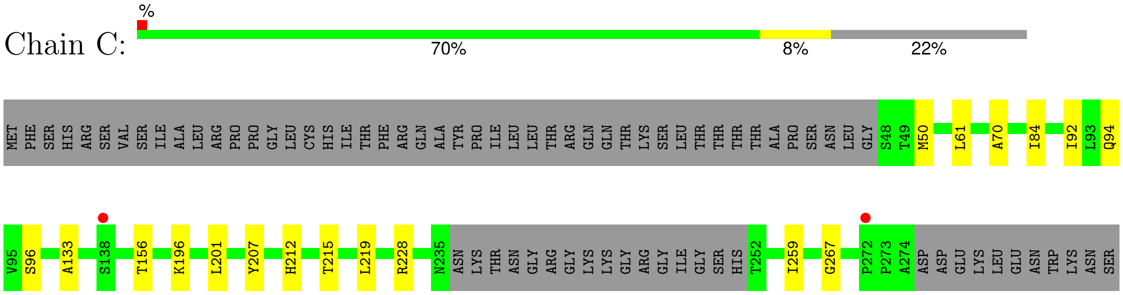
- Molecule 1: 2-oxoglutarate-dependent ethylene/succinate-forming enzyme

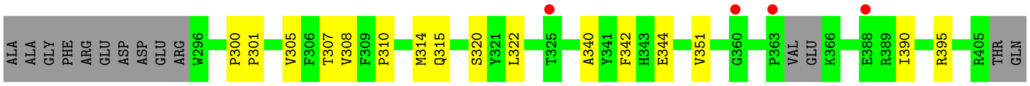
Chain B:



- Molecule 1: 2-oxoglutarate-dependent ethylene/succinate-forming enzyme

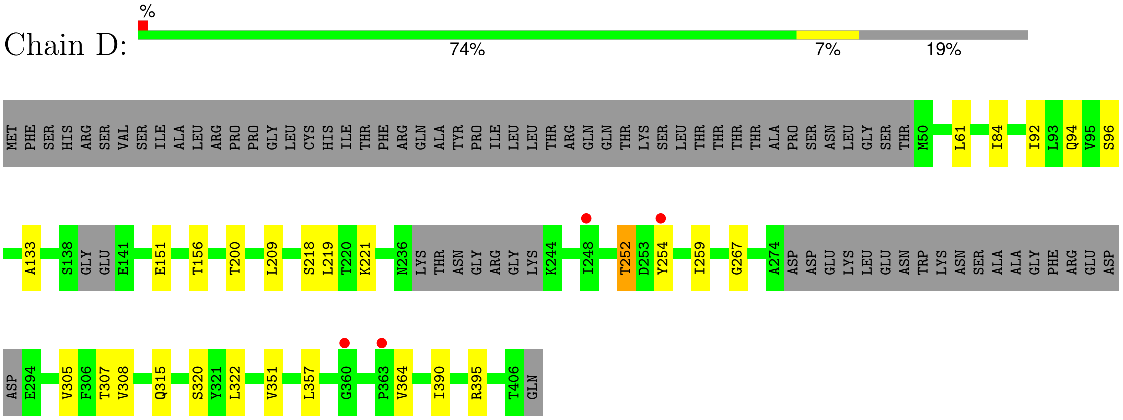
Chain C:





- Molecule 1: 2-oxoglutarate-dependent ethylene/succinate-forming enzyme

Chain D:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.60Å 115.88Å 142.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.79 – 3.50 89.79 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (89.79-3.50) 98.7 (89.79-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.242 , 0.278 0.242 , 0.279	Depositor DCC
R_{free} test set	1036 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 81.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9361	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 ⓘ

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	0.24	0/2388	0.45	0/3282
1	B	0.24	0/2333	0.44	0/3203
1	C	0.24	0/2442	0.44	0/3347
1	D	0.24	0/2486	0.44	0/3412
All	All	0.24	0/9649	0.44	0/13244

There are no bond length outliers.

There are no bond angle outliers.

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	2316	0	2074	11	0
1	B	2263	0	2065	15	0
1	C	2370	0	2174	19	0
1	D	2412	0	2213	11	0
All	All	9361	0	8526	55	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 3.

All (55) 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:96:SER:HA	1:C:305:VAL:HG12	1.71	0.71
1:D:96:SER:HA	1:D:305:VAL:HG12	1.78	0.66
1:A:96:SER:HA	1:A:305:VAL:HG12	1.79	0.64
1:C:219:LEU:HD13	1:C:351:VAL:HG12	1.80	0.63
1:C:94:GLN:HG2	1:C:307:THR:HG22	1.83	0.61
1:B:92:ILE:HD11	1:B:307:THR:HB	1.84	0.60
1:D:61:LEU:HB2	1:D:94:GLN:HE21	1.68	0.59
1:C:92:ILE:HD11	1:C:307:THR:HB	1.85	0.59
1:C:84:ILE:HG23	1:C:322:LEU:HD21	1.83	0.59
1:D:209:LEU:HD13	1:D:357:LEU:HD11	1.84	0.58
1:B:209:LEU:HD13	1:B:357:LEU:HD11	1.85	0.58
1:D:218:SER:HA	1:D:221:LYS:HE3	1.86	0.57
1:C:61:LEU:HB2	1:C:94:GLN:HE21	1.70	0.56
1:C:315:GLN:HG3	1:C:320:SER:HA	1.89	0.54
1:B:96:SER:HA	1:B:305:VAL:HG12	1.88	0.54
1:B:228:ARG:HB3	1:B:340:ALA:HB3	1.89	0.53
1:C:133:ALA:HB2	1:C:156:THR:H	1.74	0.53
1:D:92:ILE:HD11	1:D:307:THR:HB	1.91	0.52
1:D:219:LEU:HD13	1:D:351:VAL:HG12	1.92	0.52
1:B:315:GLN:HG3	1:B:320:SER:HA	1.90	0.52
1:B:84:ILE:HG23	1:B:322:LEU:HD21	1.92	0.51
1:B:219:LEU:HD13	1:B:351:VAL:HG12	1.91	0.51
1:A:259:ILE:HG12	1:A:308:VAL:HG22	1.92	0.50
1:D:84:ILE:HG23	1:D:322:LEU:HD21	1.94	0.49
1:B:94:GLN:HG2	1:B:307:THR:HG22	1.94	0.49
1:A:315:GLN:HG3	1:A:320:SER:HA	1.95	0.48
1:C:228:ARG:HB2	1:C:340:ALA:HB3	1.94	0.48
1:A:271:ARG:HB3	1:A:326:PRO:HD2	1.96	0.48
1:A:133:ALA:HB2	1:A:156:THR:H	1.79	0.46
1:A:360:GLY:O	1:C:196:LYS:HD3	2.16	0.46
1:C:201:LEU:HD13	1:C:308:VAL:HG11	1.98	0.46
1:A:201:LEU:HD13	1:A:308:VAL:HG11	1.99	0.45
1:D:390:ILE:HG23	1:D:395:ARG:HB2	1.99	0.45
1:B:133:ALA:HB2	1:B:156:THR:H	1.80	0.45
1:C:310:PRO:HB3	1:C:314:MET:HG2	2.00	0.44
1:B:128:ASP:O	1:B:386:THR:OG1	2.35	0.44
1:D:133:ALA:HB2	1:D:156:THR:H	1.83	0.44
1:A:130:GLN:HG2	1:A:389:ARG:NH1	2.33	0.44
1:A:194:LEU:HD13	1:A:341:TYR:HB2	2.00	0.43
1:D:315:GLN:HG3	1:D:320:SER:HA	2.00	0.43
1:B:194:LEU:HD22	1:B:259:ILE:HG21	2.00	0.43
1:C:342:PHE:HB3	1:C:344:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD12	1:C:94:GLN:HE21	1.84	0.43
1:C:300:PRO:HA	1:C:301:PRO:HD3	1.92	0.43
1:B:342:PHE:HB3	1:B:344:GLU:OE2	2.19	0.42
1:C:390:ILE:HG23	1:C:395:ARG:HB2	2.01	0.42
1:D:259:ILE:HG12	1:D:308:VAL:HG22	2.02	0.42
1:A:342:PHE:HB3	1:A:344:GLU:OE2	2.19	0.41
1:C:259:ILE:HG12	1:C:308:VAL:HG22	2.02	0.41
1:B:259:ILE:HG12	1:B:308:VAL:HG22	2.03	0.41
1:C:70:ALA:HB1	1:C:207:TYR:HE2	1.85	0.41
1:C:212:HIS:O	1:C:215:THR:OG1	2.27	0.41
1:B:95:VAL:HB	1:B:306:PHE:CE1	2.55	0.40
1:B:200:THR:O	1:B:204:MET:HG2	2.22	0.40
1:A:84:ILE:O	1:A:88:ARG:HG3	2.22	0.40

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	312/407 (77%)	301 (96%)	10 (3%)	1 (0%)	37	68
1	B	304/407 (75%)	292 (96%)	9 (3%)	3 (1%)	13	46
1	C	311/407 (76%)	300 (96%)	10 (3%)	1 (0%)	37	68
1	D	321/407 (79%)	304 (95%)	15 (5%)	2 (1%)	22	56
All	All	1248/1628 (77%)	1197 (96%)	44 (4%)	7 (1%)	22	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	252	THR
1	B	149	TYR

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Mol	Chain	Res	Type
1	B	150	SER
1	A	267	GLY
1	B	267	GLY
1	D	267	GLY
1	C	267	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	211/352 (60%)	207 (98%)	4 (2%)	52	73
1	B	210/352 (60%)	208 (99%)	2 (1%)	73	84
1	C	231/352 (66%)	230 (100%)	1 (0%)	89	95
1	D	229/352 (65%)	224 (98%)	5 (2%)	47	70
All	All	881/1408 (63%)	869 (99%)	12 (1%)	62	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	THR
1	A	200	THR
1	A	307	THR
1	A	321	TYR
1	B	185	THR
1	B	187	ILE
1	C	50	MET
1	D	151	GLU
1	D	200	THR
1	D	252	THR
1	D	254	TYR
1	D	364	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	94	GLN
1	D	94	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95^{th} 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	320/407 (78%)	0.21	5 (1%)	70	51	43, 70, 123, 188	0
1	B	312/407 (76%)	0.13	0	100	100	51, 73, 109, 176	0
1	C	319/407 (78%)	0.26	6 (1%)	66	46	49, 85, 135, 251	0
1	D	329/407 (80%)	0.15	4 (1%)	76	57	47, 72, 137, 213	0
All	All	1280/1628 (78%)	0.19	15 (1%)	76	57	43, 74, 126, 251	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	PRO	3.2
1	A	252	THR	2.9
1	C	272	PRO	2.8
1	C	138	SER	2.6
1	A	236	ASN	2.5
1	C	325	THR	2.5
1	C	360	GLY	2.3
1	D	360	GLY	2.3
1	D	363	PRO	2.3
1	C	388	GLU	2.3
1	D	254	TYR	2.2
1	A	254	TYR	2.1
1	D	248	ILE	2.1
1	A	156	THR	2.1
1	A	50	MET	2.0

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 (i)

There are no monosaccharides 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.