



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:51 AM JST

PDB ID : 7FF4  
Title : The crystal structure of Clostridium cellulolyticum LacI family transcriptional regulator Ccel\_1438  
Authors : Zhang, N.; Ge, H.  
Deposited on : 2021-07-22  
Resolution : 2.19 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](mailto: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>.

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

MolProbity : 4.02b-467  
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

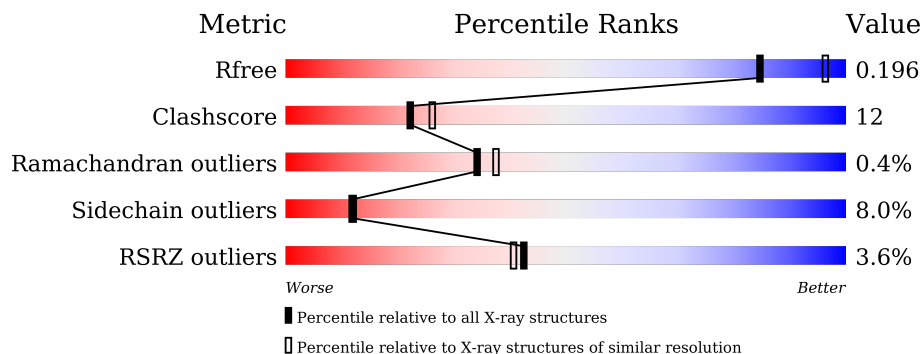
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	343	 3% 63% 14% • 18%
1	B	343	 2% 63% 15% • 19%
1	C	343	 3% 63% 12% 6% 19%
1	D	343	 3% 63% 15% • 18%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 9043 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 Transcriptional regulator, LacI family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2202	1398	374	422	8	0	0	0
1	B	278	2191	1392	372	419	8	0	0	0
1	C	279	2200	1397	373	421	9	0	1	0
1	D	280	2205	1400	374	422	9	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	HIS	-	expression tag	UNP B8I1W6
A	339	HIS	-	expression tag	UNP B8I1W6
A	340	HIS	-	expression tag	UNP B8I1W6
A	341	HIS	-	expression tag	UNP B8I1W6
A	342	HIS	-	expression tag	UNP B8I1W6
A	343	HIS	-	expression tag	UNP B8I1W6
B	338	HIS	-	expression tag	UNP B8I1W6
B	339	HIS	-	expression tag	UNP B8I1W6
B	340	HIS	-	expression tag	UNP B8I1W6
B	341	HIS	-	expression tag	UNP B8I1W6
B	342	HIS	-	expression tag	UNP B8I1W6
B	343	HIS	-	expression tag	UNP B8I1W6
C	338	HIS	-	expression tag	UNP B8I1W6
C	339	HIS	-	expression tag	UNP B8I1W6
C	340	HIS	-	expression tag	UNP B8I1W6
C	341	HIS	-	expression tag	UNP B8I1W6
C	342	HIS	-	expression tag	UNP B8I1W6
C	343	HIS	-	expression tag	UNP B8I1W6
D	338	HIS	-	expression tag	UNP B8I1W6
D	339	HIS	-	expression tag	UNP B8I1W6
D	340	HIS	-	expression tag	UNP B8I1W6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	341	HIS	-	expression tag	UNP B8I1W6
D	342	HIS	-	expression tag	UNP B8I1W6
D	343	HIS	-	expression tag	UNP B8I1W6

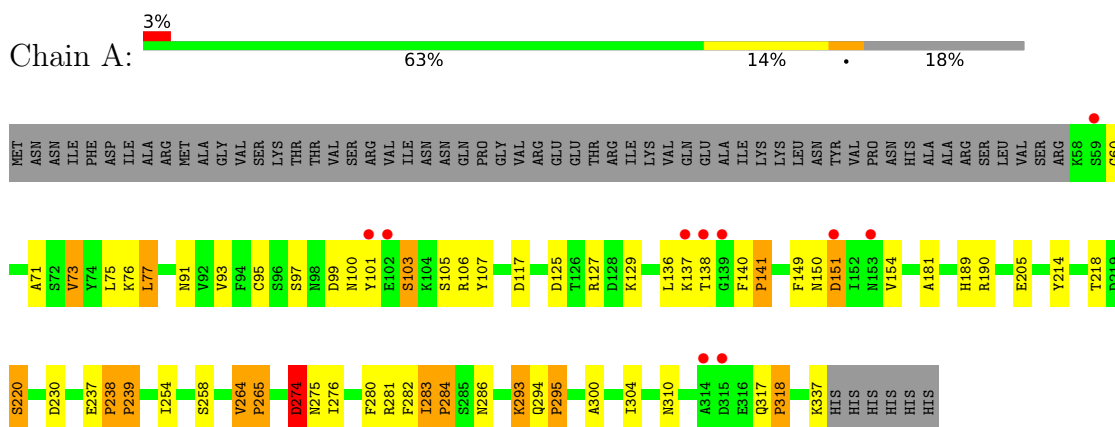
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	89	Total O 89 89	0	0
2	B	53	Total O 53 53	0	0
2	C	62	Total O 62 62	0	0
2	D	41	Total O 41 41	0	0

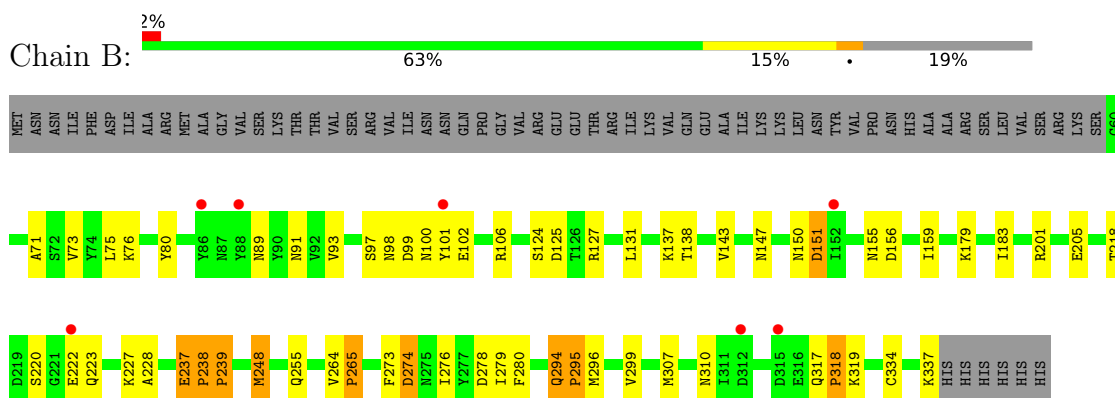
### 3 Residue-property plots [i](#)

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.

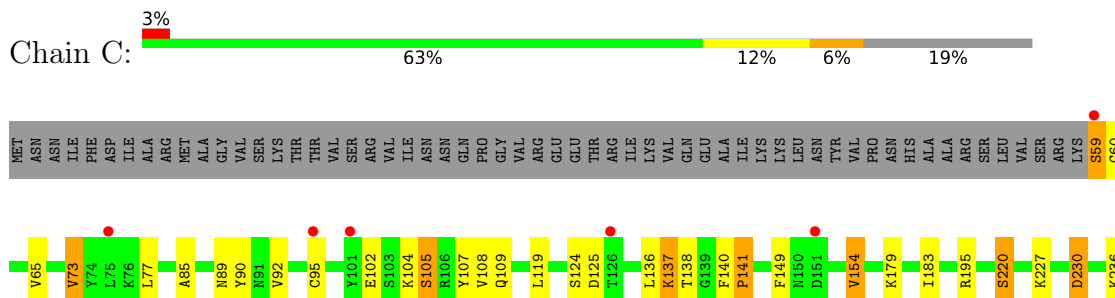
- Molecule 1: Transcriptional regulator, LacI family

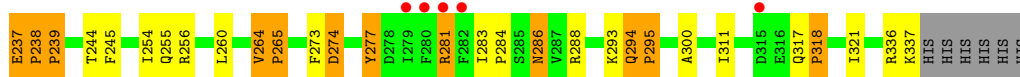


- Molecule 1: Transcriptional regulator, LacI family

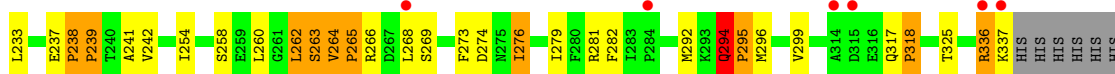
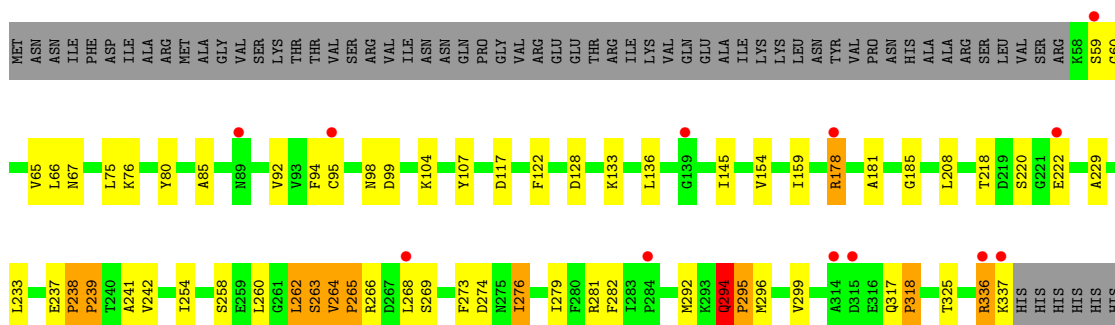


- Molecule 1: Transcriptional regulator, LacI family





- Molecule 1: Transcriptional regulator, LacI family



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.52Å 194.52Å 118.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.63 – 2.19 48.63 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.63-2.19) 99.5 (48.63-2.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.14 3260	Depositor
R, $R_{free}$	0.178 , 0.208 0.181 , 0.196	Depositor DCC
$R_{free}$ test set	4310 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.004 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$ 0.002 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.004 for $-h,2/3^*h+1/3^*k+4/3^*l,1/3^*h+2/3^*k-1/3^*l$ 0.009 for $-1/3^*h-2/3^*k+4/3^*l,-2/3^*h-1/3^*k-4/3^*l,1/3^*h-1/3^*k-1/3^*l$ 0.003 for $1/3^*h+2/3^*k-4/3^*l,-k,-2/3^*h-1/3^*k-1/3^*l$ 0.014 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	1.10	14/2242 (0.6%)	0.88	9/3035 (0.3%)
1	B	0.99	10/2231 (0.4%)	0.86	7/3020 (0.2%)
1	C	1.04	12/2243 (0.5%)	0.85	8/3036 (0.3%)
1	D	0.98	10/2248 (0.4%)	0.85	5/3043 (0.2%)
All	All	1.03	46/8964 (0.5%)	0.86	29/12134 (0.2%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	265	PRO	N-CA	13.23	1.69	1.47
1	A	141	PRO	N-CA	13.13	1.69	1.47
1	B	265	PRO	N-CA	13.13	1.69	1.47
1	D	238	PRO	N-CA	12.92	1.69	1.47
1	D	295	PRO	N-CA	12.89	1.69	1.47
1	A	284	PRO	N-CA	12.83	1.69	1.47
1	B	295	PRO	N-CA	12.82	1.69	1.47
1	C	265	PRO	N-CA	12.81	1.69	1.47
1	A	295	PRO	N-CA	12.71	1.68	1.47
1	C	141	PRO	N-CA	12.71	1.68	1.47
1	C	295	PRO	N-CA	12.67	1.68	1.47
1	A	265	PRO	N-CA	12.56	1.68	1.47
1	A	239	PRO	N-CA	12.54	1.68	1.47
1	B	318	PRO	N-CA	12.53	1.68	1.47
1	C	239	PRO	N-CA	12.52	1.68	1.47
1	D	318	PRO	N-CA	12.52	1.68	1.47
1	C	238	PRO	N-CA	12.50	1.68	1.47
1	C	318	PRO	N-CA	12.50	1.68	1.47
1	A	238	PRO	N-CA	12.48	1.68	1.47
1	A	318	PRO	N-CA	12.44	1.68	1.47
1	D	239	PRO	N-CA	12.43	1.68	1.47
1	B	238	PRO	N-CA	12.34	1.68	1.47
1	B	239	PRO	N-CA	12.17	1.68	1.47
1	D	264	VAL	C-N	5.58	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	GLU	C-N	5.55	1.44	1.34
1	B	317	GLN	C-N	5.41	1.44	1.34
1	D	238	PRO	C-N	5.41	1.44	1.34
1	D	317	GLN	C-N	5.39	1.44	1.34
1	A	283	ILE	C-N	5.38	1.44	1.34
1	A	317	GLN	C-N	5.36	1.44	1.34
1	C	140	PHE	C-N	5.32	1.44	1.34
1	C	317	GLN	C-N	5.32	1.44	1.34
1	A	140	PHE	C-N	5.32	1.44	1.34
1	C	237	GLU	C-N	5.31	1.44	1.34
1	B	294	GLN	C-N	5.29	1.44	1.34
1	C	294	GLN	C-N	5.27	1.44	1.34
1	D	294	GLN	C-N	5.26	1.44	1.34
1	B	264	VAL	C-N	5.26	1.44	1.34
1	B	237	GLU	C-N	5.26	1.44	1.34
1	C	264	VAL	C-N	5.23	1.44	1.34
1	A	237	GLU	C-N	5.20	1.44	1.34
1	A	264	VAL	C-N	5.18	1.44	1.34
1	A	294	GLN	C-N	5.15	1.44	1.34
1	B	238	PRO	C-N	5.10	1.44	1.34
1	A	238	PRO	C-N	5.07	1.43	1.34
1	C	238	PRO	C-N	5.00	1.43	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	PRO	CA-N-CD	-8.28	99.91	111.50
1	B	318	PRO	CA-N-CD	-8.12	100.14	111.50
1	D	318	PRO	CA-N-CD	-7.67	100.76	111.50
1	B	150	ASN	CB-CA-C	-7.38	95.63	110.40
1	D	265	PRO	CA-N-CD	-7.18	101.44	111.50
1	D	239	PRO	CA-N-CD	-7.16	101.47	111.50
1	C	238	PRO	CA-N-CD	-7.09	101.57	111.50
1	C	318	PRO	CA-N-CD	-7.09	101.57	111.50
1	A	238	PRO	CA-N-CD	-6.75	102.05	111.50
1	B	238	PRO	CA-N-CD	-6.71	102.11	111.50
1	A	265	PRO	CA-N-CD	-6.61	102.25	111.50
1	D	238	PRO	CA-N-CD	-6.60	102.26	111.50
1	A	284	PRO	CA-N-CD	-6.52	102.37	111.50
1	A	141	PRO	CA-N-CD	-6.34	102.63	111.50
1	A	295	PRO	CA-N-CD	-6.32	102.65	111.50
1	B	265	PRO	CA-N-CD	-6.31	102.66	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	PRO	CA-N-CD	-6.30	102.68	111.50
1	C	239	PRO	CA-N-CD	-6.28	102.71	111.50
1	C	141	PRO	CA-N-CD	-6.20	102.82	111.50
1	B	239	PRO	CA-N-CD	-6.19	102.84	111.50
1	C	295	PRO	CA-N-CD	-6.19	102.84	111.50
1	D	295	PRO	CA-N-CD	-6.13	102.91	111.50
1	C	141	PRO	N-CA-C	-5.92	96.70	112.10
1	C	265	PRO	CA-N-CD	-5.92	103.21	111.50
1	A	239	PRO	CA-N-CD	-5.89	103.25	111.50
1	A	150	ASN	CB-CA-C	-5.58	99.24	110.40
1	A	274	ASP	N-CA-CB	5.23	120.02	110.60
1	B	239	PRO	N-CA-C	-5.06	98.94	112.10
1	C	273	PHE	C-N-CA	5.01	134.21	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	2202	0	2165	63	0
1	B	2191	0	2158	53	0
1	C	2200	0	2168	50	0
1	D	2205	0	2170	58	0
2	A	89	0	0	4	0
2	B	53	0	0	0	0
2	C	62	0	0	0	0
2	D	41	0	0	0	0
All	All	9043	0	8661	205	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 12.

All (205) 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:265:PRO:CA	1:C:265:PRO:N	1.69	1.48
1:B:238:PRO:CA	1:B:238:PRO:N	1.68	1.47
1:A:284:PRO:N	1:A:284:PRO:CA	1.69	1.46
1:C:238:PRO:N	1:C:238:PRO:CA	1.68	1.46
1:A:318:PRO:N	1:A:318:PRO:CA	1.68	1.45
1:B:295:PRO:N	1:B:295:PRO:CA	1.69	1.44
1:B:265:PRO:N	1:B:265:PRO:CA	1.69	1.42
1:A:141:PRO:N	1:A:141:PRO:CA	1.69	1.42
1:D:295:PRO:N	1:D:295:PRO:CA	1.69	1.42
1:D:318:PRO:N	1:D:318:PRO:CA	1.68	1.41
1:D:238:PRO:N	1:D:238:PRO:CA	1.69	1.40
1:A:239:PRO:CA	1:A:239:PRO:N	1.68	1.39
1:C:141:PRO:N	1:C:141:PRO:CA	1.68	1.39
1:C:295:PRO:CA	1:C:295:PRO:N	1.68	1.39
1:C:239:PRO:N	1:C:239:PRO:CA	1.68	1.35
1:B:318:PRO:CA	1:B:318:PRO:N	1.68	1.34
1:D:265:PRO:CA	1:D:265:PRO:N	1.69	1.33
1:C:318:PRO:CA	1:C:318:PRO:N	1.68	1.33
1:B:239:PRO:N	1:B:239:PRO:CA	1.67	1.32
1:A:295:PRO:N	1:A:295:PRO:CA	1.68	1.32
1:D:239:PRO:N	1:D:239:PRO:CA	1.68	1.31
1:A:238:PRO:N	1:A:238:PRO:CA	1.68	1.30
1:A:265:PRO:N	1:A:265:PRO:CA	1.68	1.28
1:A:93:VAL:HG13	1:B:93:VAL:HG13	1.20	1.14
1:C:65:VAL:HA	1:C:95[B]:CYS:SG	1.89	1.12
1:D:229:ALA:O	1:D:233:LEU:HD12	1.54	1.07
1:A:293:LYS:HE2	2:A:465:HOH:O	1.53	1.06
1:D:136:LEU:HD21	1:D:154:VAL:HG12	1.33	1.03
1:D:276:ILE:HG12	1:D:279:ILE:HD12	1.40	1.02
1:D:65:VAL:HA	1:D:95[B]:CYS:SG	2.01	0.99
1:C:65:VAL:HG22	1:C:95[B]:CYS:SG	2.03	0.98
1:D:292:MET:HE2	1:D:325:THR:OG1	1.63	0.98
1:A:93:VAL:HG13	1:B:93:VAL:CG1	1.95	0.94
1:D:276:ILE:CG1	1:D:279:ILE:HD12	1.96	0.94
1:A:93:VAL:CG1	1:B:93:VAL:HG13	1.98	0.93
1:D:136:LEU:HD11	1:D:154:VAL:HG13	1.55	0.88
1:C:65:VAL:HA	1:C:95[B]:CYS:HG	1.38	0.87
1:D:136:LEU:HD11	1:D:154:VAL:CG1	2.07	0.85
1:D:65:VAL:HG22	1:D:95[B]:CYS:SG	2.16	0.84
1:D:292:MET:CE	1:D:325:THR:OG1	2.25	0.83
1:D:336:ARG:HG2	1:D:336:ARG:HH11	1.45	0.81
1:A:136:LEU:HD21	1:A:154:VAL:HG12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:HD2	1:B:205:GLU:OE1	1.82	0.79
1:C:286:ASN:OD1	1:C:286:ASN:N	2.15	0.78
1:C:136:LEU:HD11	1:C:154:VAL:HG13	1.66	0.77
1:A:282:PHE:CD1	1:B:248:MET:HG2	2.21	0.76
1:A:136:LEU:HD11	1:A:154:VAL:CG1	2.15	0.76
1:D:76:LYS:HE2	1:D:80:TYR:HE2	1.52	0.75
1:D:254:ILE:HG12	1:D:264:VAL:HG21	1.69	0.74
1:C:137:LYS:HB3	1:C:137:LYS:NZ	2.02	0.74
1:A:282:PHE:CG	1:B:248:MET:HG2	2.22	0.74
1:C:141:PRO:N	1:C:141:PRO:C	2.41	0.74
1:D:136:LEU:HD21	1:D:154:VAL:CG1	2.15	0.74
1:B:265:PRO:HB2	1:B:334:CYS:HB2	1.69	0.73
1:A:275:ASN:HB3	1:A:293:LYS:HE3	1.68	0.73
1:C:65:VAL:CA	1:C:95[B]:CYS:SG	2.73	0.72
1:A:282:PHE:HB3	1:B:248:MET:HG2	1.72	0.71
1:D:239:PRO:N	1:D:239:PRO:C	2.45	0.70
1:A:239:PRO:N	1:A:239:PRO:C	2.45	0.70
1:D:185:GLY:HA2	1:D:220:SER:HB2	1.72	0.70
1:A:91:ASN:OD1	1:B:106:ARG:NH1	2.25	0.70
1:A:205:GLU:OE1	2:A:401:HOH:O	2.09	0.70
1:B:239:PRO:N	1:B:239:PRO:C	2.44	0.70
1:C:239:PRO:N	1:C:239:PRO:C	2.45	0.70
1:A:136:LEU:HD11	1:A:154:VAL:HG13	1.75	0.69
1:C:238:PRO:N	1:C:238:PRO:C	2.45	0.69
1:B:179:LYS:HE3	1:B:237:GLU:HG2	1.75	0.68
1:C:281:ARG:HA	1:C:281:ARG:HH11	1.59	0.67
1:A:318:PRO:N	1:A:318:PRO:C	2.47	0.67
1:D:336:ARG:HH11	1:D:336:ARG:CG	2.08	0.67
1:C:136:LEU:HD21	1:C:154:VAL:HG12	1.76	0.66
1:B:238:PRO:N	1:B:238:PRO:C	2.48	0.66
1:A:238:PRO:N	1:A:238:PRO:C	2.48	0.66
1:A:141:PRO:N	1:A:141:PRO:C	2.49	0.66
1:A:106:ARG:NH1	1:B:91:ASN:OD1	2.30	0.65
1:B:318:PRO:N	1:B:318:PRO:C	2.49	0.65
1:C:73:VAL:HG13	1:C:274:ASP:HB3	1.78	0.65
1:C:65:VAL:CG2	1:C:95[B]:CYS:SG	2.82	0.65
1:A:282:PHE:CD1	1:B:248:MET:CG	2.79	0.65
1:A:286:ASN:HB3	1:B:255:GLN:NE2	2.11	0.65
1:C:137:LYS:HB3	1:C:137:LYS:HZ3	1.62	0.64
1:C:295:PRO:N	1:C:295:PRO:C	2.50	0.64
1:C:95[A]:CYS:SG	1:C:107:TYR:CD1	2.88	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:HE3	1:B:278:ASP:OD2	1.98	0.63
1:A:93:VAL:CG1	1:B:93:VAL:CG1	2.67	0.63
1:D:178:ARG:HH11	1:D:178:ARG:HG2	1.64	0.62
1:D:318:PRO:N	1:D:318:PRO:C	2.49	0.62
1:C:277:TYR:OH	1:C:284:PRO:HD2	1.99	0.62
1:D:276:ILE:HG13	1:D:279:ILE:HD12	1.80	0.62
1:A:282:PHE:CB	1:B:248:MET:HG2	2.30	0.62
1:B:295:PRO:N	1:B:295:PRO:C	2.52	0.61
1:C:283:ILE:HG22	1:C:283:ILE:O	2.01	0.60
1:A:73:VAL:HG22	2:A:411:HOH:O	2.00	0.60
1:D:238:PRO:N	1:D:238:PRO:C	2.52	0.60
1:C:318:PRO:N	1:C:318:PRO:C	2.51	0.59
1:A:295:PRO:N	1:A:295:PRO:C	2.53	0.59
1:A:100:ASN:HB3	1:A:103:SER:HB2	1.85	0.59
1:A:151:ASP:OD1	1:A:151:ASP:N	2.36	0.57
1:C:105:SER:O	1:C:109:GLN:HG3	2.04	0.57
1:C:230:ASP:OD1	1:C:256:ARG:NE	2.37	0.57
1:D:295:PRO:N	1:D:295:PRO:C	2.54	0.56
1:D:65:VAL:CA	1:D:95[B]:CYS:SG	2.87	0.56
1:A:101:TYR:HB2	1:A:127:ARG:HH11	1.71	0.56
1:D:262:LEU:HD12	1:D:263:SER:H	1.71	0.55
1:A:73:VAL:HG13	1:A:274:ASP:HB3	1.88	0.55
1:B:276:ILE:HD12	1:B:279:ILE:HD12	1.88	0.55
1:C:136:LEU:HD11	1:C:154:VAL:CG1	2.36	0.55
1:D:178:ARG:HD3	1:D:208:LEU:HD21	1.89	0.54
1:C:136:LEU:HD21	1:C:154:VAL:CG1	2.37	0.54
1:A:137:LYS:O	1:A:137:LYS:HD3	2.08	0.54
1:C:73:VAL:CG1	1:C:274:ASP:HB3	2.38	0.53
1:D:242:VAL:HG23	1:D:268:LEU:HD11	1.90	0.53
1:A:282:PHE:HA	1:B:222:GLU:HG3	1.90	0.52
1:A:280:PHE:HE1	1:B:280:PHE:CE2	2.27	0.52
1:C:277:TYR:CZ	1:C:284:PRO:HD2	2.45	0.52
1:B:220:SER:O	1:B:220:SER:OG	2.26	0.51
1:C:256:ARG:CZ	1:C:260:LEU:HD11	2.40	0.51
1:B:155:ASN:HD22	1:B:319:LYS:H	1.58	0.51
1:A:141:PRO:HA	1:A:310:ASN:HD22	1.77	0.50
1:B:151:ASP:OD1	1:B:151:ASP:N	2.40	0.50
1:A:280:PHE:CE1	1:B:280:PHE:CE2	2.99	0.50
1:A:254:ILE:HG12	1:A:264:VAL:HG11	1.94	0.49
1:D:85:ALA:CB	1:D:92:VAL:CG2	2.90	0.49
1:B:276:ILE:HD12	1:B:279:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:LYS:O	1:B:337:LYS:HG2	2.12	0.48
1:C:195:ARG:NH1	1:C:245:PHE:O	2.46	0.48
1:A:73:VAL:CG1	1:A:274:ASP:HB3	2.43	0.48
1:B:155:ASN:ND2	1:B:319:LYS:H	2.11	0.48
1:C:65:VAL:CB	1:C:95[B]:CYS:SG	3.02	0.48
1:D:181:ALA:HB2	1:D:239:PRO:HB3	1.96	0.48
1:D:65:VAL:CG2	1:D:95[B]:CYS:SG	2.97	0.48
1:D:159:ILE:HD13	1:D:294:GLN:HG2	1.96	0.48
1:A:275:ASN:HD22	1:A:293:LYS:CE	2.28	0.47
1:D:76:LYS:HE2	1:D:80:TYR:CE2	2.41	0.47
1:A:284:PRO:N	1:A:284:PRO:C	2.59	0.47
1:C:137:LYS:NZ	1:C:137:LYS:CB	2.72	0.47
1:B:143:VAL:HG23	1:B:307:MET:HE1	1.97	0.47
1:D:178:ARG:HG2	1:D:178:ARG:NH1	2.28	0.47
1:A:101:TYR:HB2	1:A:127:ARG:NH1	2.29	0.47
1:D:65:VAL:HA	1:D:95[B]:CYS:HG	1.79	0.46
1:A:283:ILE:CD1	1:B:223:GLN:HG3	2.46	0.46
1:B:127:ARG:HE	1:B:127:ARG:HB2	1.53	0.46
1:A:77:LEU:HD23	1:A:300:ALA:HB2	1.96	0.46
1:D:276:ILE:HG13	1:D:279:ILE:CD1	2.45	0.46
1:D:95[A]:CYS:SG	1:D:107:TYR:CD1	3.08	0.45
1:A:125:ASP:O	1:A:149:PHE:HZ	1.99	0.45
1:A:283:ILE:O	1:A:283:ILE:HG22	2.16	0.45
1:D:104:LYS:NZ	1:D:128:ASP:OD2	2.46	0.45
1:C:277:TYR:CD1	1:C:288:ARG:HD2	2.52	0.45
1:D:60:GLY:N	1:D:117:ASP:OD2	2.42	0.45
1:B:101:TYR:OH	1:B:131:LEU:HB2	2.16	0.45
1:B:71:ALA:HA	1:B:75:LEU:HD22	1.98	0.44
1:B:76:LYS:HD3	1:B:80:TYR:HE2	1.83	0.44
1:D:264:VAL:HG13	1:D:268:LEU:O	2.17	0.44
1:D:220:SER:O	1:D:220:SER:OG	2.33	0.44
1:D:85:ALA:CB	1:D:92:VAL:HG22	2.47	0.44
1:B:159:ILE:HD11	1:B:299:VAL:HG21	1.99	0.44
1:D:94:PHE:CD1	1:D:94:PHE:N	2.85	0.44
1:A:71:ALA:HA	1:A:75:LEU:HD22	2.00	0.43
1:A:283:ILE:HD12	1:B:223:GLN:HG3	2.00	0.43
1:A:280:PHE:HE1	1:B:280:PHE:CD2	2.36	0.43
1:C:179:LYS:NZ	1:C:237:GLU:OE1	2.37	0.43
1:A:275:ASN:HD22	1:A:293:LYS:HE3	1.83	0.43
1:B:147:ASN:O	1:B:156:ASP:OD2	2.36	0.43
1:D:136:LEU:CD2	1:D:154:VAL:HG12	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ALA:CB	1:C:92:VAL:CG2	2.97	0.43
1:D:76:LYS:NZ	1:D:296:MET:HB2	2.32	0.43
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.81	0.43
1:B:125:ASP:OD1	1:B:127:ARG:HG3	2.18	0.43
1:C:256:ARG:NH2	1:C:260:LEU:HD11	2.34	0.43
1:A:282:PHE:CD1	1:B:248:MET:HG3	2.52	0.42
1:B:75:LEU:HD12	1:B:75:LEU:HA	1.85	0.42
1:D:258:SER:HA	1:D:262:LEU:O	2.19	0.42
1:D:336:ARG:CG	1:D:336:ARG:NH1	2.72	0.42
1:B:179:LYS:CE	1:B:237:GLU:HG2	2.46	0.42
1:C:104:LYS:O	1:C:108:VAL:HG23	2.19	0.42
1:C:281:ARG:HA	1:C:281:ARG:HD2	1.49	0.42
1:A:276:ILE:HD12	1:A:276:ILE:HA	1.89	0.42
1:B:73:VAL:CG1	1:B:274:ASP:HB3	2.50	0.42
1:D:282:PHE:CD2	1:D:282:PHE:C	2.90	0.42
1:A:95:CYS:SG	1:A:107:TYR:CD1	3.07	0.42
1:A:181:ALA:HA	1:A:214:TYR:HB3	2.01	0.42
1:A:189:HIS:CD2	1:A:189:HIS:N	2.86	0.42
1:C:90:TYR:OH	1:C:311:ILE:HG21	2.19	0.41
1:D:136:LEU:CD1	1:D:154:VAL:HG13	2.37	0.41
1:C:220:SER:O	1:C:220:SER:OG	2.36	0.41
1:D:276:ILE:CG1	1:D:279:ILE:CD1	2.83	0.41
1:D:67:ASN:O	1:D:99:ASP:N	2.53	0.41
1:C:183:ILE:HD12	1:C:244:THR:HG22	2.02	0.41
1:D:75:LEU:HD12	1:D:75:LEU:HA	1.88	0.41
1:D:241:ALA:HA	1:D:269:SER:O	2.20	0.41
1:A:220:SER:O	1:A:220:SER:OG	2.39	0.41
1:A:295:PRO:HA	2:A:478:HOH:O	2.20	0.41
1:B:276:ILE:HA	1:B:279:ILE:HD12	2.03	0.41
1:C:137:LYS:CB	1:C:137:LYS:HZ2	2.34	0.41
1:B:183:ILE:HG12	1:B:228:ALA:HB1	2.02	0.41
1:B:159:ILE:HD12	1:B:295:PRO:HD2	2.02	0.41
1:C:59:SER:HB3	1:C:60:GLY:H	1.64	0.41
1:C:125:ASP:O	1:C:149:PHE:HZ	2.04	0.41
1:C:254:ILE:HG12	1:C:264:VAL:HG11	2.03	0.41
1:C:77:LEU:HD12	1:C:300:ALA:HB2	2.03	0.41
1:A:60:GLY:N	1:A:117:ASP:OD2	2.46	0.40
1:A:100:ASN:O	1:A:103:SER:HB2	2.21	0.40
1:D:66:LEU:CD2	1:D:122:PHE:CE2	3.04	0.40
1:D:295:PRO:O	1:D:299:VAL:HG23	2.21	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	278/343 (81%)	273 (98%)	4 (1%)	1 (0%)	34	37
1	B	276/343 (80%)	271 (98%)	4 (1%)	1 (0%)	34	37
1	C	278/343 (81%)	273 (98%)	4 (1%)	1 (0%)	34	37
1	D	279/343 (81%)	273 (98%)	5 (2%)	1 (0%)	34	37
All	All	1111/1372 (81%)	1090 (98%)	17 (2%)	4 (0%)	34	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	ASP
1	B	274	ASP
1	C	274	ASP
1	D	274	ASP

### 5.3.2 Protein sidechains [i](#)

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	239/296 (81%)	220 (92%)	19 (8%)	12	12
1	B	238/296 (80%)	221 (93%)	17 (7%)	14	16
1	C	240/296 (81%)	217 (90%)	23 (10%)	8	8
1	D	240/296 (81%)	223 (93%)	17 (7%)	14	16
All	All	957/1184 (81%)	881 (92%)	76 (8%)	12	12



All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	A	76	LYS
1	A	77	LEU
1	A	97	SER
1	A	99	ASP
1	A	103	SER
1	A	105	SER
1	A	129	LYS
1	A	138	THR
1	A	151	ASP
1	A	190	ARG
1	A	218	THR
1	A	220	SER
1	A	230	ASP
1	A	258	SER
1	A	281	ARG
1	A	293	LYS
1	A	304	ILE
1	A	337	LYS
1	B	89	ASN
1	B	97	SER
1	B	98	ASN
1	B	99	ASP
1	B	100	ASN
1	B	102	GLU
1	B	124	SER
1	B	137	LYS
1	B	138	THR
1	B	151	ASP
1	B	218	THR
1	B	227	LYS
1	B	248	MET
1	B	273	PHE
1	B	294	GLN
1	B	296	MET
1	B	310	ASN
1	C	59	SER
1	C	73	VAL
1	C	89	ASN
1	C	102	GLU
1	C	105	SER
1	C	119	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	124	SER
1	C	137	LYS
1	C	138	THR
1	C	154	VAL
1	C	220	SER
1	C	227	LYS
1	C	230	ASP
1	C	236	LYS
1	C	255	GLN
1	C	277	TYR
1	C	281	ARG
1	C	286	ASN
1	C	293	LYS
1	C	294	GLN
1	C	321	ILE
1	C	336	ARG
1	C	337	LYS
1	D	59	SER
1	D	98	ASN
1	D	133	LYS
1	D	145	ILE
1	D	178	ARG
1	D	218	THR
1	D	222	GLU
1	D	260	LEU
1	D	262	LEU
1	D	263	SER
1	D	266	ARG
1	D	273	PHE
1	D	276	ILE
1	D	281	ARG
1	D	294	GLN
1	D	336	ARG
1	D	337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	189	HIS
1	B	67	ASN
1	B	155	ASN
1	B	310	ASN

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Mol	Chain	Res	Type
1	D	294	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/343 (81%)	0.20	10 (3%) 42 41	35, 53, 85, 113	0
1	B	278/343 (81%)	0.12	7 (2%) 57 55	37, 57, 94, 115	0
1	C	279/343 (81%)	0.29	11 (3%) 39 37	36, 56, 87, 109	0
1	D	280/343 (81%)	0.37	12 (4%) 35 33	42, 61, 96, 121	0
All	All	1117/1372 (81%)	0.25	40 (3%) 42 41	35, 56, 92, 121	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	59	SER	6.1
1	D	337	LYS	4.9
1	B	315	ASP	4.5
1	D	139	GLY	3.6
1	A	151	ASP	3.5
1	B	86	TYR	3.5
1	B	101	TYR	3.4
1	C	101	TYR	3.3
1	D	95[A]	CYS	3.3
1	D	268	LEU	3.2
1	D	59	SER	3.1
1	A	137	LYS	3.0
1	C	126	THR	2.8
1	A	101	TYR	2.7
1	C	281	ARG	2.7
1	A	59	SER	2.6
1	C	279	ILE	2.6
1	A	139	GLY	2.5
1	A	153	ASN	2.5
1	C	151	ASP	2.5
1	D	336	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	280	PHE	2.4
1	B	312	ASP	2.4
1	D	89	ASN	2.3
1	A	138	THR	2.3
1	D	284	PRO	2.3
1	C	315	ASP	2.3
1	D	315	ASP	2.2
1	B	222	GLU	2.2
1	B	88	TYR	2.2
1	A	314	ALA	2.2
1	C	282	PHE	2.2
1	A	315	ASP	2.2
1	B	152	ILE	2.1
1	D	178	ARG	2.1
1	C	95[A]	CYS	2.1
1	C	75	LEU	2.1
1	A	102	GLU	2.0
1	D	222	GLU	2.0
1	D	314	ALA	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 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.