Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 04:22 PM EDT

PDB ID	:	2OZK
Title	:	Structure of an N-Terminal Truncated Form of Nendou (NSP15) From SARS-CORONAVIRUS
Authors	:	Saikatendu, K.; Joseph, J.; Subramanian, V.; Neuman, B.; Buchmeier, M.; Stevens, R.C.; Kuhn, P.
Deposited on	:	2007-02-26
Resolution	:	2.90 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:

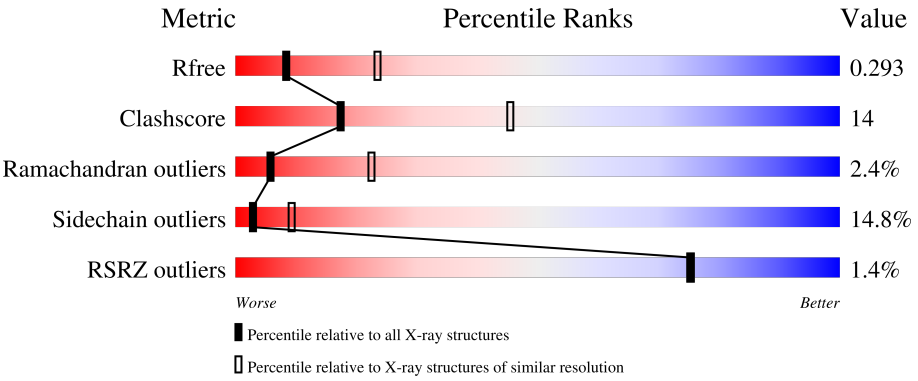
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	346	61% 23% 12%
1	B	346	61% 23% 12%
1	C	346	54% 24% 16%
1	D	346	51% 30% 5% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9402 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 Uridylate-specific endoribonuclease.

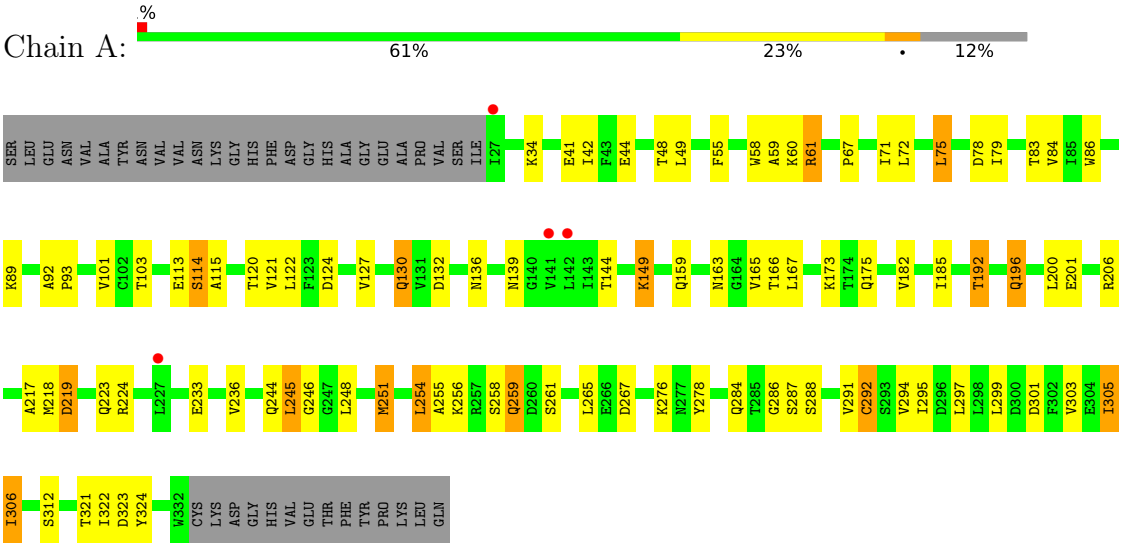
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2402	1538	391	463	10			
1	B	305	Total	C	N	O	S	0	0	0
			2394	1532	390	462	10			
1	C	291	Total	C	N	O	S	0	0	0
			2294	1473	371	440	10			
1	D	296	Total	C	N	O	S	0	0	0
			2312	1485	374	443	10			

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.

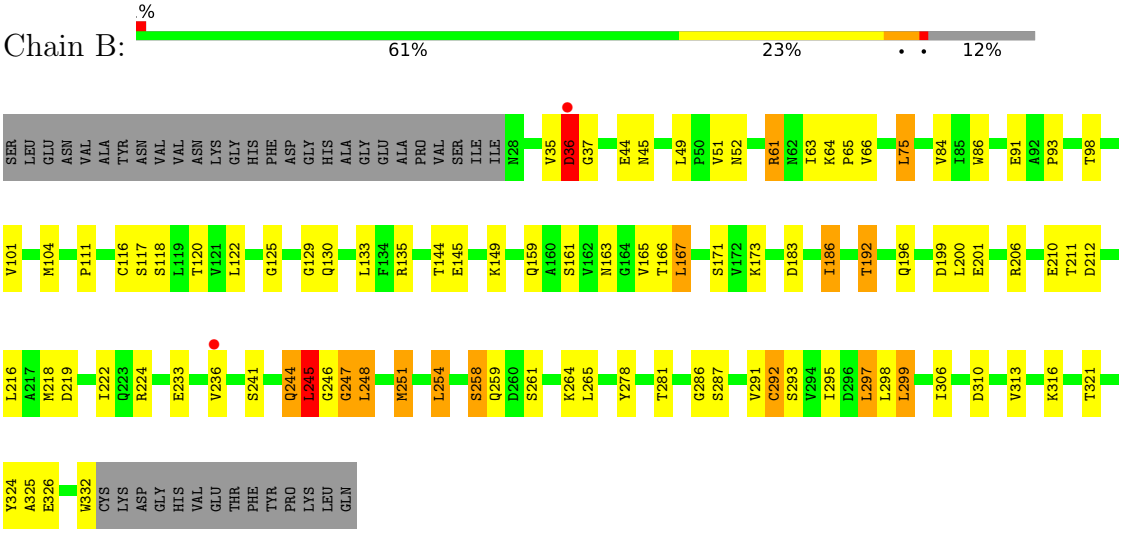
• Molecule 1: Uridylate-specific endoribonuclease

Chain A:



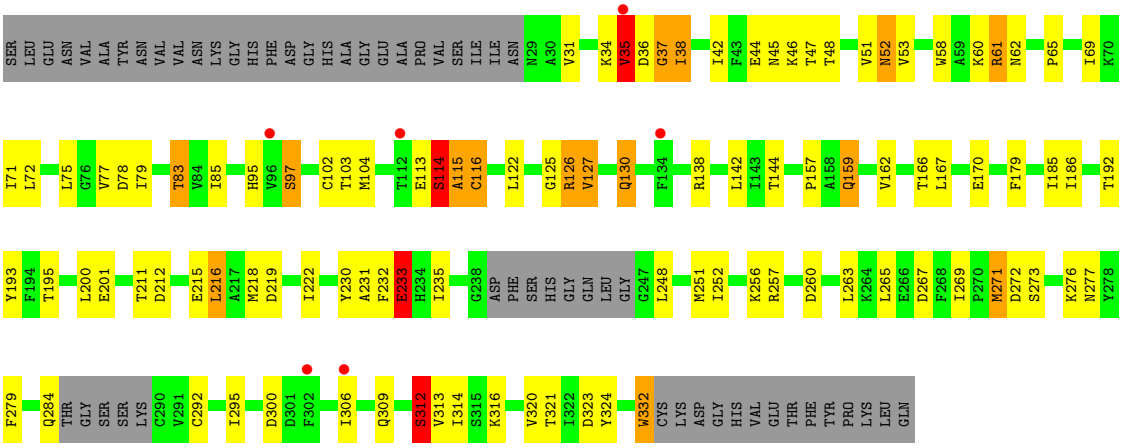
• Molecule 1: Uridylate-specific endoribonuclease

Chain B:



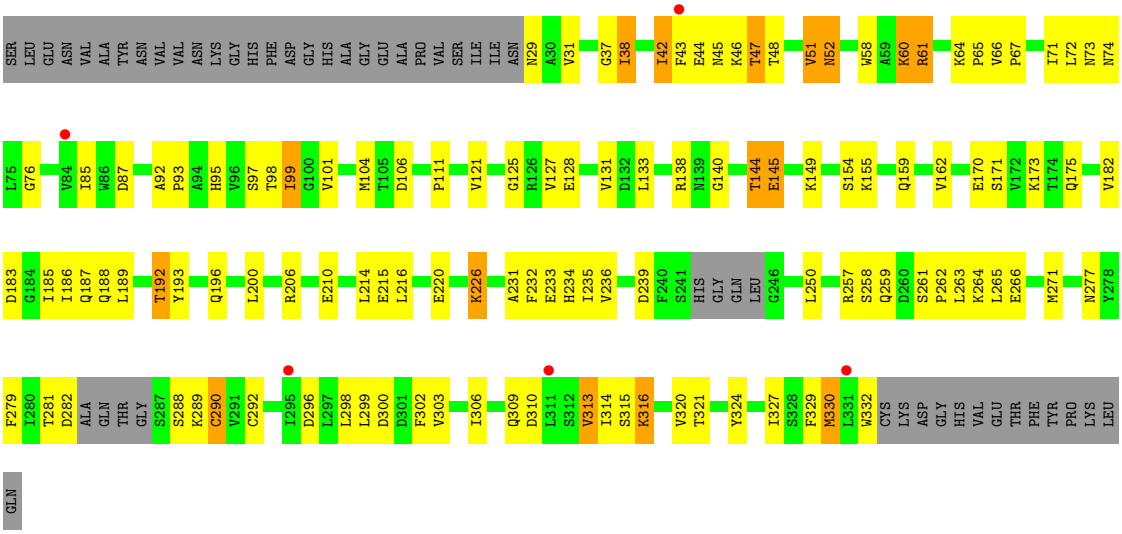
• Molecule 1: Uridylate-specific endoribonuclease

Chain C:



• Molecule 1: Uridylate-specific endoribonuclease

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	98.97Å 98.97Å 214.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.75 – 2.90 48.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.75-2.90) 97.8 (48.23-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.301 0.237 , 0.293	Depositor DCC
R_{free} test set	2601 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	73.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 20.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.448 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9402	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.55	0/2447	0.71	1/3316 (0.0%)
1	B	0.57	0/2439	0.75	2/3305 (0.1%)
1	C	0.56	0/2335	0.68	0/3163
1	D	0.56	0/2354	0.71	0/3190
All	All	0.56	0/9575	0.71	3/12974 (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
1	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	LEU	CA-CB-CG	6.84	131.04	115.30
1	A	245	LEU	CA-CB-CG	6.80	130.95	115.30
1	B	245	LEU	CA-CB-CG	6.26	129.71	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	35	VAL	Peptide

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	2402	0	2410	57	0
1	B	2394	0	2401	53	0
1	C	2294	0	2308	64	0
1	D	2312	0	2311	92	0
All	All	9402	0	9430	260	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 14.

All (260) 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:D:281:THR:HA	1:D:282:ASP:CB	1.80	1.10
1:D:281:THR:HA	1:D:282:ASP:HB2	1.12	1.05
1:D:281:THR:CA	1:D:282:ASP:HB2	1.94	0.96
1:D:192:THR:HG21	1:D:324:TYR:H	1.31	0.96
1:B:192:THR:HG21	1:B:324:TYR:H	1.31	0.92
1:C:192:THR:HG21	1:C:324:TYR:H	1.34	0.91
1:C:45:ASN:O	1:C:47:THR:N	2.03	0.91
1:D:98:THR:CG2	1:D:101:VAL:HB	2.01	0.91
1:B:35:VAL:O	1:B:36:ASP:HB3	1.73	0.89
1:D:234:HIS:CE1	1:D:239:ASP:HB3	2.10	0.86
1:D:234:HIS:HE1	1:D:239:ASP:HB3	1.41	0.85
1:B:36:ASP:OD1	1:B:37:GLY:N	2.08	0.85
1:D:98:THR:HG23	1:D:101:VAL:HB	1.55	0.84
1:D:188:GLN:O	1:D:189:LEU:HG	1.79	0.83
1:C:159:GLN:H	1:C:159:GLN:HE21	1.23	0.82
1:A:124:ASP:H	1:A:130:GLN:NE2	1.77	0.81
1:A:301:ASP:O	1:A:305:ILE:HG23	1.82	0.79
1:D:315:SER:HB3	1:D:330:MET:HE1	1.65	0.78
1:D:31:VAL:HG22	1:D:52:ASN:HB2	1.66	0.78
1:D:44:GLU:CB	1:D:45:ASN:HA	2.14	0.77
1:C:309:GLN:HE21	1:C:316:LYS:HD3	1.49	0.77
1:C:312:SER:HB2	1:C:314:ILE:N	2.02	0.75
1:A:192:THR:HG21	1:A:324:TYR:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:THR:HG23	1:D:321:THR:HG22	1.69	0.73
1:C:312:SER:HB2	1:C:313:VAL:CA	2.18	0.73
1:B:61:ARG:NH1	1:B:163:ASN:ND2	2.36	0.73
1:B:61:ARG:HH12	1:B:163:ASN:ND2	1.86	0.73
1:D:314:ILE:O	1:D:316:LYS:NZ	2.22	0.72
1:D:98:THR:HG22	1:D:106:ASP:HB3	1.70	0.72
1:C:312:SER:HB2	1:C:313:VAL:C	2.09	0.72
1:C:192:THR:HG22	1:C:193:TYR:O	1.90	0.72
1:B:61:ARG:NH1	1:B:163:ASN:HD21	1.89	0.70
1:B:192:THR:CG2	1:B:324:TYR:H	2.04	0.70
1:B:291:VAL:O	1:B:292:CYS:HB3	1.91	0.70
1:A:58:TRP:O	1:A:61:ARG:HG3	1.91	0.70
1:D:316:LYS:HB2	1:D:316:LYS:HZ3	1.57	0.69
1:C:44:GLU:HB3	1:C:45:ASN:O	1.93	0.69
1:A:61:ARG:HG2	1:A:86:TRP:HB2	1.73	0.69
1:C:277:ASN:HA	1:C:292:CYS:O	1.93	0.68
1:B:61:ARG:HH12	1:B:163:ASN:HD21	1.40	0.68
1:D:281:THR:CA	1:D:282:ASP:CB	2.64	0.68
1:D:316:LYS:NZ	1:D:316:LYS:HB2	2.08	0.68
1:C:51:VAL:HG23	1:C:52:ASN:H	1.59	0.67
1:C:312:SER:HB3	1:C:316:LYS:NZ	2.11	0.65
1:D:98:THR:HG21	1:D:101:VAL:HB	1.78	0.65
1:C:45:ASN:C	1:C:47:THR:H	1.96	0.65
1:B:259:GLN:HA	1:B:259:GLN:OE1	1.96	0.65
1:D:234:HIS:HE1	1:D:239:ASP:CB	2.08	0.65
1:B:192:THR:HG21	1:B:324:TYR:N	2.09	0.65
1:A:284:GLN:OE1	1:B:63:ILE:HG12	1.96	0.64
1:D:309:GLN:HB3	1:D:316:LYS:HD3	1.78	0.64
1:B:295:ILE:HG12	1:B:297:LEU:HD23	1.78	0.64
1:C:65:PRO:HB3	1:C:162:VAL:HG22	1.80	0.64
1:C:127:VAL:HG23	1:C:130:GLN:HG3	1.79	0.64
1:A:276:LYS:HB3	1:A:278:TYR:CE1	2.34	0.63
1:D:235:ILE:HD11	1:D:302:PHE:HZ	1.64	0.63
1:D:289:LYS:H	1:D:290:CYS:HA	1.64	0.63
1:D:315:SER:HB3	1:D:330:MET:CE	2.29	0.62
1:B:245:LEU:HD23	1:D:329:PHE:HA	1.80	0.62
1:B:196:GLN:HE21	1:B:206:ARG:HD2	1.64	0.61
1:A:127:VAL:CG2	1:A:130:GLN:HG3	2.30	0.61
1:D:303:VAL:HA	1:D:306:ILE:HD12	1.81	0.61
1:B:111:PRO:HD2	1:B:133:LEU:HD22	1.83	0.61
1:D:37:GLY:HA2	1:D:38:ILE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:HB3	1:D:45:ASN:CA	2.31	0.61
1:D:192:THR:CG2	1:D:324:TYR:H	2.11	0.60
1:C:65:PRO:O	1:C:126:ARG:NH2	2.33	0.60
1:D:192:THR:HG22	1:D:193:TYR:O	2.01	0.60
1:C:212:ASP:HB3	1:C:216:LEU:HD23	1.83	0.60
1:D:44:GLU:CB	1:D:45:ASN:CA	2.80	0.60
1:D:95:HIS:HD2	1:D:97:SER:O	1.83	0.60
1:A:192:THR:HG21	1:A:324:TYR:N	2.16	0.60
1:C:159:GLN:H	1:C:159:GLN:NE2	1.98	0.60
1:D:196:GLN:HE21	1:D:206:ARG:HH11	1.48	0.60
1:C:257:ARG:O	1:C:260:ASP:O	2.20	0.59
1:A:259:GLN:HE21	1:A:259:GLN:N	2.00	0.59
1:C:71:ILE:CD1	1:C:157:PRO:HG2	2.32	0.59
1:C:65:PRO:HB3	1:C:162:VAL:CG2	2.32	0.59
1:D:186:ILE:HD12	1:D:186:ILE:H	1.68	0.59
1:D:125:GLY:HA2	1:D:131:VAL:HG22	1.86	0.58
1:A:127:VAL:HG23	1:A:130:GLN:HG3	1.86	0.58
1:A:259:GLN:HE21	1:A:259:GLN:H	1.51	0.58
1:D:51:VAL:HG23	1:D:52:ASN:H	1.69	0.58
1:D:65:PRO:HB3	1:D:162:VAL:HG22	1.85	0.57
1:B:129:GLY:O	1:B:133:LEU:HD12	2.05	0.57
1:B:241:SER:HB3	1:B:248:LEU:HB2	1.87	0.57
1:D:37:GLY:HA2	1:D:38:ILE:HG13	1.84	0.57
1:A:196:GLN:HG3	1:A:206:ARG:HH11	1.69	0.57
1:B:295:ILE:HG12	1:B:297:LEU:CD2	2.34	0.57
1:C:58:TRP:O	1:C:61:ARG:HB3	2.04	0.56
1:C:31:VAL:HG22	1:C:52:ASN:HB2	1.86	0.56
1:D:316:LYS:N	1:D:330:MET:HE1	2.20	0.56
1:C:69:ILE:HA	1:C:72:LEU:HD12	1.88	0.55
1:A:61:ARG:NH1	1:A:163:ASN:ND2	2.54	0.55
1:C:51:VAL:HG23	1:C:52:ASN:N	2.21	0.55
1:C:231:ALA:O	1:C:233:GLU:N	2.39	0.55
1:C:312:SER:HB2	1:C:313:VAL:HA	1.87	0.55
1:A:124:ASP:H	1:A:130:GLN:HE22	1.55	0.55
1:A:124:ASP:N	1:A:130:GLN:HE21	2.04	0.55
1:B:196:GLN:HE21	1:B:206:ARG:HH11	1.55	0.55
1:D:231:ALA:O	1:D:233:GLU:N	2.34	0.54
1:B:254:LEU:O	1:B:258:SER:HB2	2.07	0.54
1:C:142:LEU:HD21	1:C:144:THR:HG23	1.90	0.54
1:C:312:SER:HB3	1:C:316:LYS:HZ2	1.71	0.54
1:D:196:GLN:HE21	1:D:206:ARG:NH1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:N	1:A:130:GLN:NE2	2.50	0.53
1:D:235:ILE:HD11	1:D:302:PHE:CZ	2.43	0.53
1:D:309:GLN:HE21	1:D:316:LYS:HG2	1.72	0.53
1:A:41:GLU:OE2	1:A:44:GLU:HB2	2.08	0.53
1:A:265:LEU:HD23	1:A:278:TYR:CG	2.44	0.53
1:A:192:THR:HG21	1:A:324:TYR:HA	1.91	0.52
1:D:44:GLU:HB3	1:D:45:ASN:C	2.29	0.52
1:D:42:ILE:O	1:D:51:VAL:HG22	2.10	0.52
1:D:277:ASN:HA	1:D:292:CYS:O	2.10	0.52
1:D:66:VAL:HB	1:D:67:PRO:HD2	1.91	0.52
1:D:258:SER:HB2	1:D:263:LEU:H	1.75	0.52
1:D:44:GLU:HB2	1:D:45:ASN:HA	1.90	0.52
1:B:130:GLN:HA	1:B:133:LEU:HD12	1.92	0.52
1:D:47:THR:O	1:D:48:THR:HB	2.09	0.52
1:D:170:GLU:HG2	1:D:171:SER:N	2.25	0.52
1:D:196:GLN:HB2	1:D:296:ASP:OD1	2.09	0.52
1:D:200:LEU:HD23	1:D:265:LEU:HD22	1.91	0.52
1:A:79:ILE:HG23	1:A:121:VAL:HG22	1.91	0.52
1:C:230:TYR:O	1:C:313:VAL:HG23	2.09	0.52
1:A:139:ASN:OD1	1:A:182:VAL:O	2.28	0.51
1:D:155:LYS:HE2	1:D:175:GLN:OE1	2.10	0.51
1:A:61:ARG:NH1	1:A:163:ASN:HD21	2.09	0.51
1:B:244:GLN:HG3	1:B:248:LEU:HG	1.92	0.51
1:D:210:GLU:HG2	1:D:299:LEU:HB2	1.93	0.50
1:D:92:ALA:HB1	1:D:93:PRO:CD	2.42	0.50
1:B:218:MET:HE3	1:B:222:ILE:HG23	1.94	0.50
1:D:95:HIS:CD2	1:D:97:SER:O	2.64	0.50
1:D:288:SER:HB2	1:D:290:CYS:HB3	1.93	0.50
1:A:86:TRP:CZ3	1:A:93:PRO:HD3	2.46	0.50
1:C:271:MET:CG	1:C:272:ASP:H	2.24	0.50
1:C:312:SER:CB	1:C:313:VAL:HA	2.42	0.49
1:C:142:LEU:C	1:C:142:LEU:HD23	2.32	0.49
1:B:212:ASP:O	1:B:216:LEU:HG	2.12	0.49
1:D:125:GLY:HA3	1:D:144:THR:HG23	1.94	0.49
1:C:211:THR:O	1:C:215:GLU:HG2	2.13	0.49
1:A:67:PRO:HG2	1:A:72:LEU:HD11	1.93	0.49
1:B:244:GLN:CD	1:B:244:GLN:H	2.16	0.48
1:A:165:VAL:HG21	1:B:201:GLU:HB2	1.96	0.48
1:A:201:GLU:HB3	1:B:165:VAL:HG21	1.95	0.48
1:A:265:LEU:HD23	1:A:278:TYR:CD2	2.48	0.48
1:B:219:ASP:HA	1:B:222:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LEU:HA	1:D:279:PHE:O	2.13	0.48
1:B:246:GLY:HA3	1:B:292:CYS:HA	1.94	0.48
1:D:44:GLU:HB3	1:D:46:LYS:N	2.29	0.48
1:D:99:ILE:HA	1:D:106:ASP:HB2	1.96	0.48
1:B:125:GLY:HA3	1:B:144:THR:HG22	1.94	0.48
1:C:195:THR:OG1	1:C:323:ASP:OD2	2.23	0.48
1:D:182:VAL:HG23	1:D:187:GLN:HG3	1.96	0.47
1:B:145:GLU:HB2	1:B:173:LYS:HD2	1.97	0.47
1:D:60:LYS:HE3	1:D:101:VAL:O	2.15	0.47
1:D:183:ASP:C	1:D:185:ILE:H	2.17	0.47
1:A:124:ASP:H	1:A:130:GLN:HE21	1.52	0.47
1:C:248:LEU:HD21	1:C:295:ILE:HG22	1.96	0.47
1:A:60:LYS:HD3	1:A:101:VAL:HG13	1.96	0.47
1:A:61:ARG:HH11	1:A:163:ASN:ND2	2.13	0.47
1:D:289:LYS:N	1:D:290:CYS:HA	2.30	0.47
1:D:58:TRP:O	1:D:61:ARG:HB3	2.15	0.46
1:D:74:ASN:C	1:D:76:GLY:H	2.19	0.46
1:A:255:ALA:O	1:A:258:SER:HB2	2.16	0.46
1:C:72:LEU:O	1:C:77:VAL:HG23	2.16	0.46
1:D:236:VAL:HG22	1:D:250:LEU:HD21	1.96	0.46
1:A:79:ILE:CG2	1:A:121:VAL:HG22	2.46	0.46
1:B:216:LEU:HD11	1:B:224:ARG:NH2	2.31	0.46
1:B:310:ASP:O	1:B:313:VAL:HG22	2.15	0.46
1:C:125:GLY:HA3	1:C:144:THR:HG22	1.96	0.46
1:C:114:SER:O	1:C:116:CYS:N	2.49	0.46
1:C:218:MET:O	1:C:222:ILE:HG13	2.16	0.46
1:D:85:ILE:H	1:D:95:HIS:CE1	2.34	0.46
1:C:44:GLU:HB3	1:C:45:ASN:CA	2.46	0.46
1:C:79:ILE:HG23	1:C:95:HIS:CD2	2.52	0.45
1:C:142:LEU:HD22	1:C:179:PHE:CD1	2.51	0.45
1:D:67:PRO:HG2	1:D:72:LEU:HD21	1.98	0.45
1:B:61:ARG:NH1	1:B:63:ILE:HG22	2.31	0.45
1:B:84:VAL:HG23	1:B:101:VAL:HG11	1.98	0.45
1:A:113:GLU:O	1:A:115:ALA:N	2.50	0.45
1:C:312:SER:CB	1:C:313:VAL:CA	2.91	0.45
1:A:192:THR:HG21	1:A:324:TYR:CA	2.47	0.45
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.77	0.45
1:B:196:GLN:NE2	1:B:206:ARG:HH11	2.15	0.45
1:C:95:HIS:HD2	1:C:97:SER:O	2.00	0.45
1:D:263:LEU:HD23	1:D:282:ASP:HA	1.99	0.45
1:B:286:GLY:O	1:B:287:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASP:HB3	1:C:216:LEU:CD2	2.47	0.45
1:D:144:THR:HG22	1:D:145:GLU:OE2	2.16	0.45
1:A:200:LEU:HD13	1:A:251:MET:CE	2.47	0.44
1:B:332:TRP:HZ3	1:D:271:MET:HG3	1.82	0.44
1:C:159:GLN:HE21	1:C:159:GLN:N	2.04	0.44
1:D:261:SER:N	1:D:262:PRO:HD3	2.32	0.44
1:A:58:TRP:C	1:A:60:LYS:H	2.21	0.44
1:A:113:GLU:O	1:A:114:SER:C	2.56	0.44
1:A:75:LEU:HD13	1:A:75:LEU:HA	1.88	0.44
1:D:281:THR:HA	1:D:282:ASP:HB3	1.88	0.44
1:A:83:THR:OG1	1:A:84:VAL:N	2.51	0.44
1:C:51:VAL:CG2	1:C:52:ASN:H	2.27	0.44
1:A:71:ILE:HG22	1:A:75:LEU:HD23	2.00	0.43
1:D:309:GLN:HB3	1:D:316:LYS:CD	2.45	0.43
1:A:132:ASP:O	1:A:136:ASN:ND2	2.51	0.43
1:A:286:GLY:O	1:A:287:SER:C	2.56	0.43
1:D:92:ALA:HB1	1:D:93:PRO:HD2	2.00	0.43
1:A:58:TRP:O	1:A:60:LYS:N	2.52	0.43
1:A:92:ALA:HB1	1:A:93:PRO:HD2	2.00	0.43
1:C:62:ASN:HD22	1:C:83:THR:HG21	1.83	0.43
1:B:86:TRP:CZ3	1:B:93:PRO:HD3	2.53	0.43
1:B:210:GLU:HG2	1:B:299:LEU:HB2	2.00	0.43
1:A:149:LYS:O	1:A:149:LYS:HG2	2.19	0.43
1:C:37:GLY:HA2	1:C:38:ILE:HA	1.67	0.43
1:C:71:ILE:HD12	1:C:157:PRO:HG2	2.00	0.43
1:C:231:ALA:HB1	1:C:332:TRP:HA	2.01	0.43
1:B:316:LYS:H	1:D:73:ASN:HD22	1.67	0.43
1:D:216:LEU:HD23	1:D:220:GLU:HB3	2.00	0.43
1:A:278:TYR:O	1:A:291:VAL:HA	2.19	0.42
1:B:75:LEU:HD12	1:B:75:LEU:HA	1.66	0.42
1:C:85:ILE:H	1:C:95:HIS:HE1	1.67	0.42
1:A:301:ASP:O	1:A:305:ILE:CG2	2.62	0.42
1:D:258:SER:HB2	1:D:263:LEU:N	2.33	0.42
1:D:320:VAL:HG22	1:D:321:THR:N	2.35	0.42
1:C:85:ILE:H	1:C:95:HIS:CE1	2.37	0.42
1:D:48:THR:HG22	1:D:48:THR:O	2.19	0.42
1:D:264:LYS:HB3	1:D:281:THR:O	2.19	0.42
1:B:278:TYR:O	1:B:291:VAL:HA	2.20	0.42
1:D:43:PHE:O	1:D:51:VAL:HG13	2.20	0.42
1:D:111:PRO:HG2	1:D:133:LEU:HD23	2.01	0.42
1:A:294:VAL:HG12	1:A:295:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:CYS:C	1:B:118:SER:H	2.24	0.42
1:B:321:THR:HA	1:B:325:ALA:O	2.20	0.42
1:D:87:ASP:OD1	1:D:87:ASP:C	2.58	0.42
1:D:214:LEU:HG	1:D:259:GLN:HE22	1.85	0.42
1:B:61:ARG:NH1	1:B:63:ILE:CG2	2.83	0.42
1:C:45:ASN:C	1:C:47:THR:N	2.64	0.42
1:D:121:VAL:H	1:D:140:GLY:HA2	1.85	0.42
1:D:154:SER:HB2	1:D:189:LEU:HD13	2.02	0.42
1:C:313:VAL:HG22	1:C:313:VAL:O	2.20	0.41
1:C:48:THR:O	1:C:48:THR:HG22	2.19	0.41
1:A:217:ALA:O	1:A:218:MET:C	2.59	0.41
1:A:322:ILE:O	1:A:323:ASP:HB2	2.20	0.41
1:A:246:GLY:HA3	1:A:292:CYS:HA	2.02	0.41
1:B:186:ILE:HD13	1:B:186:ILE:HA	1.91	0.41
1:B:247:GLY:N	1:B:292:CYS:HB2	2.35	0.41
1:C:34:LYS:O	1:C:35:VAL:C	2.59	0.41
1:C:216:LEU:O	1:C:256:LYS:NZ	2.51	0.41
1:B:200:LEU:HD13	1:B:251:MET:HE1	2.02	0.41
1:C:44:GLU:HB3	1:C:45:ASN:HA	2.02	0.41
1:A:256:LYS:O	1:A:259:GLN:NE2	2.51	0.41
1:A:42:ILE:HD12	1:A:55:PHE:HE1	1.86	0.41
1:D:258:SER:HB3	1:D:263:LEU:HD12	2.02	0.41
1:B:135:ARG:NH2	1:B:149:LYS:O	2.49	0.41
1:C:312:SER:HB3	1:C:316:LYS:HZ3	1.86	0.41
1:C:71:ILE:CD1	1:C:157:PRO:CG	2.97	0.40
1:A:219:ASP:O	1:A:223:GLN:HB2	2.21	0.40
1:A:303:VAL:HA	1:A:306:ILE:HG23	2.01	0.40
1:B:64:LYS:HB3	1:B:65:PRO:CD	2.51	0.40
1:B:91:GLU:O	1:B:91:GLU:HG3	2.21	0.40
1:C:44:GLU:HB3	1:C:45:ASN:C	2.42	0.40
1:C:114:SER:HB2	1:C:115:ALA:H	1.62	0.40
1:D:98:THR:HG22	1:D:106:ASP:CB	2.46	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	304/346 (88%)	267 (88%)	34 (11%)	3 (1%)	15 45
1	B	303/346 (88%)	271 (89%)	27 (9%)	5 (2%)	9 31
1	C	285/346 (82%)	240 (84%)	32 (11%)	13 (5%)	2 9
1	D	290/346 (84%)	247 (85%)	36 (12%)	7 (2%)	6 22
All	All	1182/1384 (85%)	1025 (87%)	129 (11%)	28 (2%)	6 22

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	46	LYS
1	C	115	ALA
1	C	232	PHE
1	D	52	ASN
1	D	232	PHE
1	D	310	ASP
1	D	313	VAL
1	A	59	ALA
1	A	61	ARG
1	A	114	SER
1	B	247	GLY
1	C	35	VAL
1	C	36	ASP
1	C	114	SER
1	C	116	CYS
1	C	312	SER
1	D	38	ILE
1	D	226	LYS
1	C	37	GLY
1	C	52	ASN
1	C	233	GLU
1	D	149	LYS
1	B	36	ASP
1	B	171	SER
1	B	292	CYS
1	B	117	SER
1	C	38	ILE
1	C	126	ARG

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	270/303 (89%)	230 (85%)	40 (15%)	3 9
1	B	269/303 (89%)	229 (85%)	40 (15%)	3 9
1	C	258/303 (85%)	212 (82%)	46 (18%)	2 5
1	D	258/303 (85%)	228 (88%)	30 (12%)	5 16
All	All	1055/1212 (87%)	899 (85%)	156 (15%)	3 9

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	48	THR
1	A	49	LEU
1	A	75	LEU
1	A	78	ASP
1	A	89	LYS
1	A	103	THR
1	A	120	THR
1	A	122	LEU
1	A	130	GLN
1	A	144	THR
1	A	149	LYS
1	A	159	GLN
1	A	166	THR
1	A	167	LEU
1	A	173	LYS
1	A	175	GLN
1	A	185	ILE
1	A	192	THR
1	A	196	GLN
1	A	219	ASP
1	A	224	ARG
1	A	233	GLU
1	A	236	VAL

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	245	LEU
1	A	248	LEU
1	A	251	MET
1	A	254	LEU
1	A	259	GLN
1	A	261	SER
1	A	267	ASP
1	A	288	SER
1	A	292	CYS
1	A	297	LEU
1	A	299	LEU
1	A	305	ILE
1	A	306	ILE
1	A	312	SER
1	A	321	THR
1	B	36	ASP
1	B	44	GLU
1	B	45	ASN
1	B	49	LEU
1	B	51	VAL
1	B	52	ASN
1	B	61	ARG
1	B	66	VAL
1	B	75	LEU
1	B	98	THR
1	B	104	MET
1	B	120	THR
1	B	122	LEU
1	B	159	GLN
1	B	161	SER
1	B	166	THR
1	B	167	LEU
1	B	183	ASP
1	B	186	ILE
1	B	192	THR
1	B	199	ASP
1	B	211	THR
1	B	233	GLU
1	B	236	VAL
1	B	244	GLN
1	B	245	LEU

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	251	MET
1	B	254	LEU
1	B	258	SER
1	B	261	SER
1	B	264	LYS
1	B	265	LEU
1	B	281	THR
1	B	293	SER
1	B	297	LEU
1	B	298	LEU
1	B	299	LEU
1	B	306	ILE
1	B	326	GLU
1	C	42	ILE
1	C	53	VAL
1	C	60	LYS
1	C	61	ARG
1	C	75	LEU
1	C	78	ASP
1	C	83	THR
1	C	97	SER
1	C	102	CYS
1	C	103	THR
1	C	104	MET
1	C	113	GLU
1	C	114	SER
1	C	122	LEU
1	C	127	VAL
1	C	130	GLN
1	C	138	ARG
1	C	159	GLN
1	C	166	THR
1	C	167	LEU
1	C	170	GLU
1	C	185	ILE
1	C	186	ILE
1	C	200	LEU
1	C	201	GLU
1	C	216	LEU
1	C	219	ASP
1	C	233	GLU

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Mol	Chain	Res	Type
1	C	235	ILE
1	C	251	MET
1	C	252	ILE
1	C	263	LEU
1	C	265	LEU
1	C	267	ASP
1	C	269	ILE
1	C	271	MET
1	C	273	SER
1	C	276	LYS
1	C	279	PHE
1	C	284	GLN
1	C	300	ASP
1	C	306	ILE
1	C	312	SER
1	C	320	VAL
1	C	321	THR
1	C	332	TRP
1	D	29	ASN
1	D	42	ILE
1	D	47	THR
1	D	51	VAL
1	D	60	LYS
1	D	61	ARG
1	D	64	LYS
1	D	71	ILE
1	D	99	ILE
1	D	104	MET
1	D	127	VAL
1	D	128	GLU
1	D	138	ARG
1	D	144	THR
1	D	145	GLU
1	D	159	GLN
1	D	173	LYS
1	D	192	THR
1	D	215	GLU
1	D	226	LYS
1	D	257	ARG
1	D	266	GLU
1	D	290	CYS
1	D	298	LEU

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Mol	Chain	Res	Type
1	D	300	ASP
1	D	313	VAL
1	D	316	LYS
1	D	327	ILE
1	D	330	MET
1	D	332	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	130	GLN
1	A	159	GLN
1	A	163	ASN
1	A	259	GLN
1	B	45	ASN
1	B	163	ASN
1	B	175	GLN
1	B	196	GLN
1	B	234	HIS
1	C	52	ASN
1	C	62	ASN
1	C	73	ASN
1	C	95	HIS
1	C	130	GLN
1	C	159	GLN
1	C	249	HIS
1	C	259	GLN
1	C	309	GLN
1	D	29	ASN
1	D	73	ASN
1	D	82	ASN
1	D	95	HIS
1	D	130	GLN
1	D	196	GLN
1	D	234	HIS
1	D	259	GLN
1	D	309	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 monosaccharides 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	306/346 (88%)	0.28	4 (1%)	77	77	48, 63, 79, 86	0
1	B	305/346 (88%)	0.29	2 (0%)	87	87	47, 63, 79, 82	0
1	C	291/346 (84%)	0.39	6 (2%)	63	61	50, 78, 95, 103	0
1	D	296/346 (85%)	0.36	5 (1%)	70	69	55, 77, 95, 104	0
All	All	1198/1384 (86%)	0.33	17 (1%)	75	75	47, 70, 92, 104	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	THR	3.4
1	D	311	LEU	2.9
1	C	134	PHE	2.9
1	D	331	LEU	2.3
1	C	96	VAL	2.3
1	C	306	ILE	2.2
1	B	36	ASP	2.1
1	A	227	LEU	2.1
1	A	142	LEU	2.1
1	B	236	VAL	2.1
1	D	295	ILE	2.1
1	C	35	VAL	2.1
1	A	27	ILE	2.1
1	A	141	VAL	2.1
1	D	84	VAL	2.0
1	D	43	PHE	2.0
1	C	302	PHE	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.