



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:47 AM GMT

PDB ID : 3PV2  
Title : Structure of Legionella fallonii DegQ (wt)  
Authors : Wrase, R.; Scott, H.; Hilgenfeld, R.; Hansen, G.  
Deposited on : 2010-12-06  
Resolution : 2.15 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

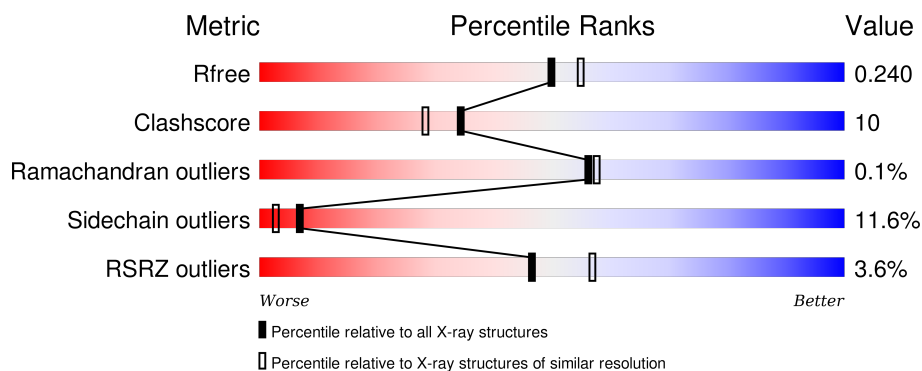
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	451	<div> <div>2%</div> <div>67% 14% • 15%</div> </div>
1	B	451	<div> <div>2%</div> <div>71% 12% • 14%</div> </div>
1	C	451	<div> <div>6%</div> <div>66% 17% • 14%</div> </div>
1	D	451	<div> <div>2%</div> <div>65% 16% • 15%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12098 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 DegQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	4	0
			2895	1838	504	546	7			
1	B	388	Total	C	N	O	S	0	4	0
			2925	1856	509	554	6			
1	C	388	Total	C	N	O	S	0	4	0
			2922	1852	512	551	7			
1	D	383	Total	C	N	O	S	0	4	0
			2888	1833	502	546	7			

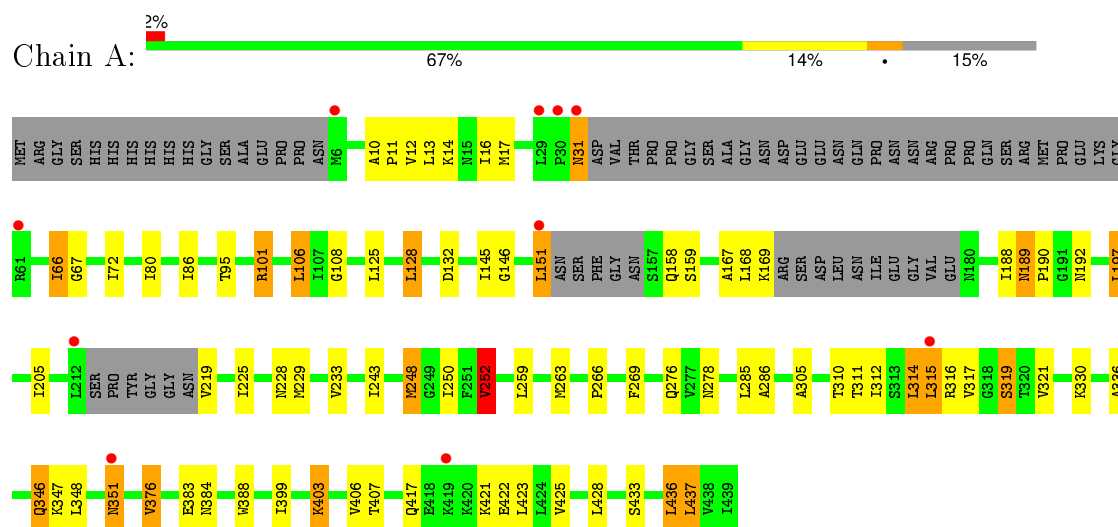
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	128	Total	O	0	0
			128	128		
2	C	105	Total	O	0	0
			105	105		
2	D	112	Total	O	0	0
			112	112		

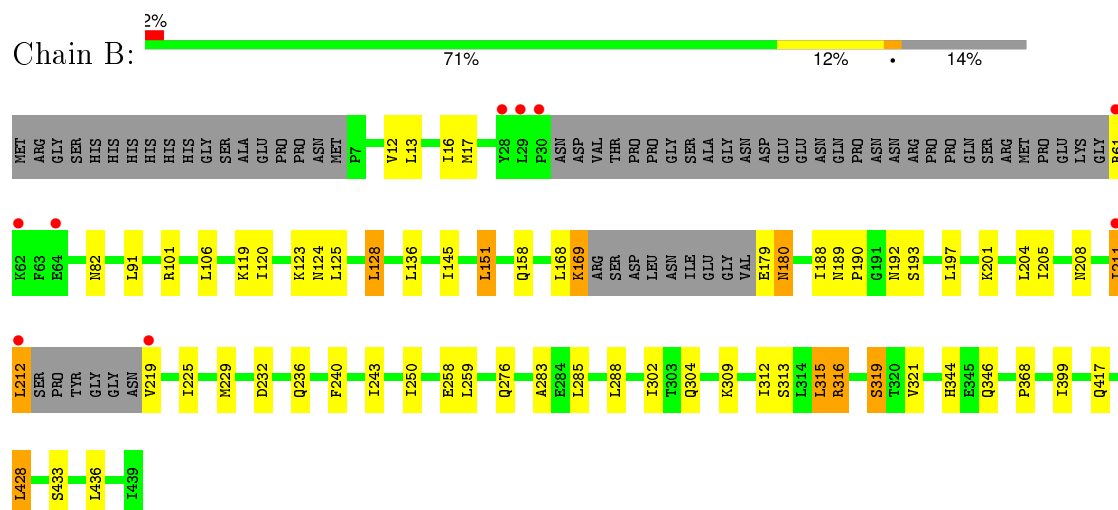
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DegQ

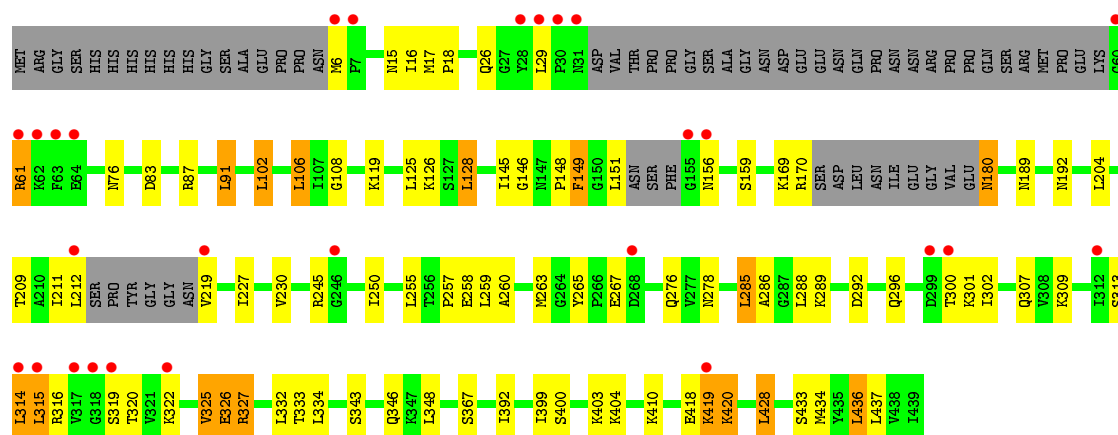


#### • Molecule 1: DegQ

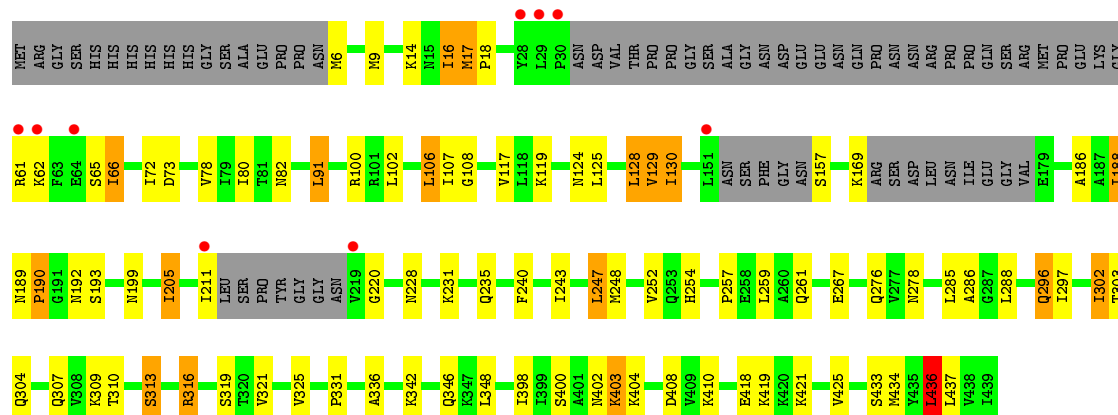


#### • Molecule 1: DegQ





• Molecule 1: DegQ



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.70Å 136.70Å 327.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.93 – 2.15 36.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.93-2.15) 98.1 (36.93-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.211 , 0.251 0.202 , 0.240	Depositor DCC
$R_{free}$ test set	6107 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.6	EDS
Estimated twinning fraction	0.004 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.005 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.007 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.003 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.004 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.002 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.018 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 121556 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.04	0/2932	1.00	4/3971 (0.1%)
1	B	1.01	0/2964	0.95	1/4015 (0.0%)
1	C	0.93	0/2959	0.91	2/4006 (0.0%)
1	D	0.95	0/2925	0.94	1/3961 (0.0%)
All	All	0.98	0/11780	0.95	8/15953 (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	A	145	ILE	CB-CA-C	-5.73	100.13	111.60
1	C	327	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	C	102	LEU	CA-CB-CG	5.51	127.98	115.30
1	D	436	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	436	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	101	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	252	VAL	CG1-CB-CG2	5.17	119.17	110.90
1	A	101	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	2895	0	3022	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2925	0	3044	40	0
1	C	2922	0	3047	62	0
1	D	2888	0	3011	65	0
2	A	123	0	0	0	0
2	B	128	0	0	2	0
2	C	105	0	0	4	0
2	D	112	0	0	4	0
All	All	12098	0	12124	237	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 10.

All (237) 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:72:ILE:HD13	1:D:80:ILE:CD1	1.74	1.17
1:A:72:ILE:CD1	1:A:80:ILE:HD11	1.74	1.16
1:A:72:ILE:HD13	1:A:80:ILE:HD11	1.19	1.11
1:D:72:ILE:HD13	1:D:80:ILE:HD11	1.32	1.08
1:A:72:ILE:HD13	1:A:80:ILE:CD1	1.86	1.04
1:D:398:ILE:HG23	1:D:425:VAL:CG2	1.93	0.98
1:B:428:LEU:HD12	1:B:433:SER:OG	1.65	0.96
1:D:276:GLN:HE21	1:D:278:ASN:HD21	1.06	0.93
1:A:399:ILE:HD13	1:A:428:LEU:CD1	1.99	0.93
1:B:250:ILE:O	1:B:250:ILE:HG13	1.68	0.90
1:D:72:ILE:CD1	1:D:80:ILE:HD11	2.03	0.88
1:D:189[B]:ASN:HB2	1:D:192:ASN:ND2	1.88	0.87
1:D:303:THR:H	1:D:307:GLN:NE2	1.72	0.86
1:A:399:ILE:HD13	1:A:428:LEU:HD11	1.57	0.85
1:D:72:ILE:HD13	1:D:80:ILE:HD12	1.59	0.83
1:C:322:LYS:HE3	1:C:333:THR:HG22	1.61	0.82
1:A:312:ILE:HA	1:A:315:LEU:HD22	1.60	0.81
1:D:72:ILE:CD1	1:D:80:ILE:CD1	2.58	0.81
1:D:303:THR:H	1:D:307:GLN:HE22	1.30	0.80
1:A:72:ILE:CD1	1:A:80:ILE:CD1	2.51	0.78
1:C:250:ILE:HG21	1:C:288:LEU:HD23	1.65	0.78
1:D:276:GLN:HE21	1:D:278:ASN:ND2	1.82	0.78
1:A:31:ASN:H	1:A:31:ASN:HD22	1.30	0.78
1:A:197:LEU:HD13	1:A:205:ILE:HD11	1.66	0.77
1:A:31:ASN:HD22	1:A:31:ASN:N	1.83	0.77
1:A:233:VAL:HG13	1:A:243:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLN:HE21	1:B:243:ILE:HA	1.51	0.75
1:A:189[B]:ASN:HB2	1:A:192:ASN:ND2	2.03	0.74
1:D:398:ILE:HG23	1:D:425:VAL:HG21	1.68	0.73
1:C:148:PRO:HD3	1:C:192:ASN:HD21	1.54	0.72
1:C:316:ARG:O	1:C:319:SER:HB3	1.88	0.72
1:C:276:GLN:HE21	1:C:278:ASN:HD21	1.38	0.72
1:A:189[B]:ASN:HB2	1:A:192:ASN:HD22	1.55	0.72
1:A:197:LEU:HD13	1:A:205:ILE:CD1	2.22	0.70
1:C:315:LEU:HD21	1:C:319:SER:OG	1.91	0.70
1:D:9:MET:HA	1:D:9:MET:CE	2.23	0.69
1:A:189[A]:ASN:HD21	1:A:192:ASN:HD22	1.40	0.68
1:B:17:MET:HG2	1:B:158:GLN:NE2	2.09	0.67
1:A:276:GLN:HE21	1:A:278:ASN:HD21	1.40	0.66
1:C:392:ILE:HG13	1:C:436:LEU:HD23	1.76	0.66
1:B:151:LEU:HD13	1:B:151:LEU:O	1.95	0.66
1:B:236:GLN:HG2	1:B:243:ILE:CD1	2.25	0.66
1:D:189[B]:ASN:HB2	1:D:192:ASN:HD21	1.60	0.66
1:A:276:GLN:NE2	1:A:278:ASN:HD21	1.94	0.65
1:B:236:GLN:HG2	1:B:243:ILE:HD13	1.78	0.65
1:A:252:VAL:HG13	1:A:305:ALA:HB1	1.79	0.65
1:D:316:ARG:O	1:D:319:SER:HB3	1.96	0.65
1:C:322:LYS:HE3	1:C:333:THR:CG2	2.27	0.65
1:A:399:ILE:CD1	1:A:428:LEU:CD1	2.74	0.64
1:C:106:LEU:HD22	1:C:108:GLY:N	2.13	0.64
1:D:404:LYS:HE3	1:D:418:GLU:OE2	1.96	0.64
1:A:399:ILE:HD13	1:A:428:LEU:HD13	1.79	0.64
1:A:225:ILE:HG23	1:A:229:MET:HE1	1.80	0.63
1:C:76:ASN:O	1:C:119:LYS:HE3	1.98	0.63
1:D:309:LYS:O	1:D:313:SER:HB2	1.99	0.63
1:C:314:LEU:C	1:C:314:LEU:HD23	2.19	0.63
1:B:312:ILE:HA	1:B:315:LEU:HD22	1.81	0.62
1:C:309:LYS:O	1:C:313:SER:N	2.26	0.62
1:B:236:GLN:NE2	1:B:243:ILE:HG23	2.15	0.62
1:A:66:ILE:HD12	1:A:67:GLY:N	2.14	0.61
1:D:304:GLN:H	1:D:307:GLN:HE21	1.49	0.61
1:C:314:LEU:C	1:C:314:LEU:CD2	2.69	0.60
1:D:128:LEU:H	1:D:128:LEU:HD12	1.66	0.60
1:B:250:ILE:HG21	1:B:288:LEU:CD2	2.31	0.60
1:C:315:LEU:CD2	1:C:319:SER:OG	2.50	0.60
1:C:399:ILE:HG21	1:C:428:LEU:HD22	1.82	0.60
1:C:289:LYS:HG2	1:C:327:ARG:NH2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:HG3	1:C:180:ASN:HD21	1.67	0.59
1:B:309:LYS:O	1:B:313:SER:HB3	2.03	0.59
1:D:186:ALA:O	1:D:188[A]:ILE:HD12	2.02	0.59
1:A:422:GLU:HB2	1:A:437:LEU:CD2	2.33	0.58
1:B:16:ILE:HD11	1:B:145:ILE:HD11	1.84	0.58
1:A:146:GLY:HA3	1:A:192:ASN:OD1	2.03	0.58
1:A:72:ILE:HD11	1:A:80:ILE:HD11	1.76	0.57
1:D:220:GLY:HA2	2:D:450:HOH:O	2.04	0.57
1:B:399:ILE:HD13	1:B:428:LEU:HD13	1.87	0.57
1:D:72:ILE:CD1	1:D:80:ILE:HD12	2.32	0.57
1:A:266:PRO:HD2	1:A:269:PHE:HB2	1.86	0.57
1:D:261:GLN:NE2	1:D:267:GLU:HB2	2.19	0.57
1:A:72:ILE:CG2	1:A:80:ILE:HD12	2.35	0.56
1:B:136:LEU:HD21	1:B:205:ILE:HD13	1.88	0.56
1:B:189[B]:ASN:HB2	1:B:192:ASN:ND2	2.20	0.56
1:C:258:GLU:HG3	1:D:100:ARG:HG3	1.86	0.56
1:B:250:ILE:HG21	1:B:288:LEU:HD23	1.88	0.56
1:D:189[B]:ASN:HB2	1:D:192:ASN:HD22	1.68	0.56
1:C:29:LEU:HD12	1:C:61:ARG:HG3	1.88	0.56
1:C:320:THR:HG23	2:C:489:HOH:O	2.05	0.56
1:C:227:ILE:HD12	1:C:230:VAL:HB	1.87	0.55
1:C:296:GLN:HA	1:C:302:ILE:HD12	1.89	0.55
1:B:250:ILE:CG2	1:B:283:ALA:CB	2.85	0.55
1:C:419:LYS:HG3	1:C:420:LYS:N	2.21	0.55
1:A:106:LEU:HD22	1:A:108:GLY:N	2.22	0.55
1:A:106:LEU:CD2	1:A:108:GLY:N	2.71	0.54
1:B:211:ILE:O	1:B:212:LEU:HB3	2.07	0.54
1:B:188[A]:ILE:HD12	1:B:208:ASN:HB3	1.90	0.54
1:A:403:LYS:HZ2	1:C:263:MET:HE2	1.73	0.54
1:A:286:ALA:HB2	1:A:336:ALA:HB2	1.89	0.54
1:A:72:ILE:HG12	1:A:80:ILE:HD12	1.90	0.54
1:D:72:ILE:HG21	1:D:80:ILE:HD12	1.90	0.54
1:D:398:ILE:CG2	1:D:425:VAL:CG2	2.78	0.53
1:B:344:HIS:ND1	2:B:547:HOH:O	2.33	0.53
1:D:106:LEU:HD22	1:D:108:GLY:H	1.72	0.53
1:D:107:ILE:HD12	1:D:117:VAL:HG12	1.91	0.53
1:C:146:GLY:HA3	1:C:192:ASN:HD22	1.73	0.53
1:D:402:ASN:O	1:D:403:LYS:HB2	2.09	0.53
1:A:403:LYS:NZ	1:C:263:MET:HE2	2.23	0.53
1:D:106:LEU:HD22	1:D:108:GLY:N	2.24	0.53
1:C:265:TYR:HE2	1:C:326:GLU:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ILE:CG2	1:D:425:VAL:HG21	2.38	0.52
1:A:403:LYS:NZ	1:C:263:MET:CE	2.72	0.52
1:A:72:ILE:CG1	1:A:80:ILE:CD1	2.88	0.52
1:A:189[A]:ASN:HB2	1:A:190[A]:PRO:HD2	1.92	0.52
1:C:286:ALA:O	1:C:334:LEU:HD22	2.10	0.52
1:A:399:ILE:CD1	1:A:428:LEU:HD11	2.36	0.51
1:A:311:THR:O	1:A:315:LEU:HD13	2.10	0.51
1:B:250:ILE:HG23	1:B:283:ALA:CB	2.40	0.51
1:C:17:MET:N	1:C:18:PRO:CD	2.73	0.51
1:C:276:GLN:NE2	1:C:278:ASN:HD21	2.05	0.51
2:C:521:HOH:O	1:D:6:MET:HE1	2.09	0.51
1:C:292:ASP:HB3	1:C:325:VAL:CG2	2.41	0.51
1:D:189[B]:ASN:O	1:D:190[B]:PRO:C	2.48	0.51
1:C:322:LYS:CE	1:C:333:THR:HG22	2.37	0.51
1:A:72:ILE:CG1	1:A:80:ILE:HD12	2.41	0.50
1:C:428:LEU:HD12	1:C:433:SER:OG	2.11	0.50
1:A:128:LEU:HD12	1:A:128:LEU:N	2.26	0.50
1:C:146:GLY:HA3	1:C:192:ASN:ND2	2.27	0.50
1:B:13:LEU:O	1:B:17:MET:HG3	2.11	0.50
1:A:189[A]:ASN:C	1:A:189[A]:ASN:HD22	2.16	0.49
1:D:128:LEU:N	1:D:128:LEU:HD12	2.26	0.49
1:C:245:ARG:HG2	1:C:313:SER:O	2.12	0.49
1:B:240:PHE:CZ	1:B:316:ARG:HD2	2.47	0.49
1:A:422:GLU:HB2	1:A:437:LEU:HD22	1.95	0.49
1:C:292:ASP:HB3	1:C:325:VAL:HG21	1.95	0.49
1:B:179:GLU:HG2	1:B:180:ASN:H	1.78	0.49
1:A:422:GLU:HB2	1:A:437:LEU:HD21	1.94	0.49
1:A:106:LEU:CD2	1:A:108:GLY:H	2.25	0.48
1:D:130:ILE:HD11	1:D:231:LYS:CD	2.43	0.48
1:D:17:MET:HB2	1:D:18:PRO:HD3	1.95	0.48
1:D:240:PHE:CE2	1:D:316:ARG:HD2	2.48	0.48
1:B:428:LEU:CD1	1:B:433:SER:OG	2.50	0.48
1:D:276:GLN:NE2	1:D:278:ASN:HD21	1.90	0.48
1:A:259:LEU:O	1:A:263:MET:HG3	2.13	0.48
1:A:421:LYS:HG3	1:A:422:GLU:HG2	1.95	0.48
1:A:310:THR:O	1:A:314:LEU:HD22	2.14	0.47
1:A:248:MET:HG3	1:A:312:ILE:HG21	1.96	0.47
1:A:31:ASN:ND2	1:A:31:ASN:N	2.55	0.47
1:B:82:ASN:ND2	1:B:193:SER:OG	2.47	0.47
1:A:403:LYS:HZ2	1:C:263:MET:CE	2.27	0.47
1:D:129:VAL:HG13	2:D:512:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG23	1:A:229:MET:CE	2.44	0.47
1:C:29:LEU:HD12	1:C:61:ARG:CG	2.45	0.47
1:B:128:LEU:HD12	1:B:128:LEU:N	2.30	0.47
1:A:167:ALA:O	1:A:168:LEU:HD23	2.15	0.47
1:A:72:ILE:HG21	1:A:80:ILE:HD12	1.96	0.47
1:A:128:LEU:HD12	1:A:128:LEU:H	1.80	0.47
1:A:384:ASN:HA	1:D:91:LEU:HD11	1.97	0.47
1:C:250:ILE:HG21	1:C:288:LEU:CD2	2.40	0.46
1:D:304:GLN:N	1:D:307:GLN:HE21	2.11	0.46
1:C:327:ARG:HG3	1:C:332:LEU:HD12	1.97	0.46
1:A:376:VAL:HG13	1:A:406:VAL:CG1	2.46	0.46
1:C:128:LEU:HD21	1:C:204:LEU:HB2	1.98	0.46
1:C:106:LEU:HD22	1:C:108:GLY:H	1.79	0.46
1:A:146:GLY:CA	1:A:192:ASN:OD1	2.64	0.46
1:D:247:LEU:HG	1:D:248:MET:N	2.29	0.46
1:C:189[B]:ASN:HB2	1:C:192:ASN:OD1	2.16	0.46
1:C:209:THR:HG22	1:C:211:ILE:HG12	1.97	0.46
1:D:9:MET:HA	1:D:9:MET:HE3	1.96	0.45
1:A:219:VAL:HG22	1:A:219:VAL:O	2.15	0.45
1:B:399:ILE:CD1	1:B:428:LEU:HD13	2.45	0.45
1:A:316:ARG:O	1:A:319:SER:OG	2.24	0.45
1:A:72:ILE:HG12	1:A:80:ILE:CD1	2.47	0.45
1:B:128:LEU:HD12	1:B:128:LEU:H	1.81	0.45
1:A:132:ASP:HA	1:A:228:ASN:HD21	1.82	0.45
1:C:128:LEU:CD2	1:C:204:LEU:HB2	2.47	0.45
1:D:248:MET:HE1	1:D:321:VAL:HG11	1.99	0.44
1:D:254:HIS:HD2	2:D:482:HOH:O	2.01	0.44
1:D:297:ILE:HG13	1:D:302:ILE:HD13	1.98	0.44
1:A:13:LEU:O	1:A:17:MET:HG2	2.17	0.44
1:C:320:THR:CG2	2:C:489:HOH:O	2.64	0.44
1:D:321:VAL:HG12	1:D:336:ALA:O	2.17	0.44
1:C:170:ARG:HG3	1:C:180:ASN:ND2	2.30	0.44
1:B:258:GLU:HG3	2:B:508:HOH:O	2.18	0.44
1:A:189[A]:ASN:HB2	1:A:190[A]:PRO:CD	2.48	0.44
1:C:148:PRO:HG2	1:C:149:PHE:CE2	2.53	0.43
1:C:91:LEU:HD23	2:C:519:HOH:O	2.18	0.43
1:D:9:MET:HA	1:D:9:MET:HE2	1.97	0.43
1:D:73:ASP:HB3	1:D:78:VAL:HB	2.00	0.43
1:D:296:GLN:HE21	1:D:296:GLN:HB2	1.70	0.43
1:A:225:ILE:CG2	1:A:229:MET:CE	2.96	0.43
1:A:86:ILE:HD12	1:A:86:ILE:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:N	1:A:151:LEU:CD1	2.81	0.43
1:B:168:LEU:O	1:B:169:LYS:HB3	2.17	0.43
1:A:347:LYS:O	1:A:351:ASN:HB3	2.19	0.43
1:D:72:ILE:CG2	1:D:80:ILE:HD12	2.49	0.42
1:C:419:LYS:HG3	1:C:420:LYS:H	1.81	0.42
1:D:199:ASN:N	1:D:205:ILE:CD1	2.83	0.42
1:B:225:ILE:CG2	1:B:229:MET:HE2	2.49	0.42
1:A:10:ALA:N	1:A:11:PRO:CD	2.83	0.42
1:C:400:SER:HB2	1:C:404:LYS:O	2.20	0.42
1:B:316:ARG:O	1:B:319:SER:OG	2.36	0.42
1:C:434:MET:HG2	1:C:436:LEU:HD13	2.01	0.42
1:B:201:LYS:HD2	1:C:6:MET:SD	2.60	0.42
1:B:428:LEU:HD12	1:B:433:SER:HG	1.75	0.42
1:A:189[B]:ASN:O	1:A:190[B]:PRO:C	2.57	0.42
1:C:309:LYS:HG2	1:C:313:SER:HB2	2.01	0.42
1:C:302:ILE:HA	1:C:307:GLN:OE1	2.19	0.42
1:A:346:GLN:HE21	1:A:346:GLN:HA	1.85	0.42
1:B:236:GLN:HG2	1:B:243:ILE:HD12	2.01	0.41
1:D:408:ASP:HB2	2:D:541:HOH:O	2.20	0.41
1:A:276:GLN:HE21	1:A:278:ASN:ND2	2.14	0.41
1:A:276:GLN:NE2	1:A:278:ASN:ND2	2.66	0.41
1:D:16:ILE:HG22	1:D:128:LEU:HB3	2.00	0.41
1:B:180:ASN:OD1	1:B:180:ASN:C	2.58	0.41
1:B:128:LEU:HD22	1:B:204:LEU:HB2	2.03	0.41
1:C:83:ASP:OD1	1:C:87:ARG:NH1	2.47	0.41
1:D:82:ASN:ND2	1:D:193:SER:OG	2.53	0.41
1:B:16:ILE:HD11	1:B:145:ILE:CD1	2.50	0.41
1:C:418:GLU:CG	1:C:419:LYS:N	2.83	0.41
1:C:418:GLU:HG2	1:C:419:LYS:H	1.85	0.41
1:D:107:ILE:HD11	1:D:119:LYS:HB2	2.03	0.41
1:D:400:SER:O	1:D:425:VAL:HG23	2.20	0.41
1:A:151:LEU:HD13	1:A:151:LEU:N	2.36	0.41
1:A:250:ILE:HG21	1:A:250:ILE:HD13	1.85	0.41
1:D:434:MET:HE3	1:D:436:LEU:HD11	2.02	0.41
1:D:398:ILE:HG23	1:D:425:VAL:HG23	1.90	0.41
1:D:286:ALA:HB2	1:D:336:ALA:HB2	2.03	0.41
1:A:95:THR:OG1	1:A:101:ARG:HD2	2.21	0.41
1:D:325:VAL:O	1:D:331:PRO:HA	2.21	0.41
1:D:228:ASN:HA	1:D:231:LYS:HE3	2.03	0.41
1:C:15:ASN:HD22	1:C:15:ASN:HA	1.72	0.41
1:C:257:PRO:O	1:C:260:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:HD22	1:C:285:LEU:O	2.21	0.40
1:D:66:ILE:CD1	1:D:66:ILE:N	2.84	0.40
1:A:188[B]:ILE:HA	1:A:188[B]:ILE:HD13	1.92	0.40
1:A:383:GLU:HA	1:A:388:TRP:CG	2.57	0.40
1:B:119:LYS:HG3	1:B:120:ILE:N	2.37	0.40
1:D:303:THR:N	1:D:307:GLN:NE2	2.55	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	378/451 (84%)	373 (99%)	5 (1%)	0	100	100
1	B	384/451 (85%)	376 (98%)	6 (2%)	2 (0%)	34	26
1	C	382/451 (85%)	369 (97%)	13 (3%)	0	100	100
1	D	377/451 (84%)	370 (98%)	5 (1%)	2 (0%)	34	26
All	All	1521/1804 (84%)	1488 (98%)	29 (2%)	4 (0%)	56	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	190[A]	PRO
1	D	190[B]	PRO
1	B	190[A]	PRO
1	B	190[B]	PRO

### 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	319/372 (86%)	283 (89%)	36 (11%)	7	3
1	B	322/372 (87%)	292 (91%)	30 (9%)	11	6
1	C	321/372 (86%)	282 (88%)	39 (12%)	6	2
1	D	318/372 (86%)	274 (86%)	44 (14%)	4	1
All	All	1280/1488 (86%)	1131 (88%)	149 (12%)	7	3

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	14	LYS
1	A	16	ILE
1	A	31	ASN
1	A	66	ILE
1	A	106	LEU
1	A	125	LEU
1	A	128	LEU
1	A	151	LEU
1	A	158	GLN
1	A	159	SER
1	A	169	LYS
1	A	189[A]	ASN
1	A	189[B]	ASN
1	A	197	LEU
1	A	248	MET
1	A	252	VAL
1	A	285	LEU
1	A	314	LEU
1	A	315	LEU
1	A	317	VAL
1	A	319	SER
1	A	321	VAL
1	A	330	LYS
1	A	346	GLN
1	A	348	LEU
1	A	351	ASN
1	A	376	VAL

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Mol	Chain	Res	Type
1	A	403	LYS
1	A	407	THR
1	A	417	GLN
1	A	423	LEU
1	A	425	VAL
1	A	433	SER
1	A	436	LEU
1	A	437	LEU
1	B	12	VAL
1	B	61	ARG
1	B	91	LEU
1	B	106	LEU
1	B	123	LYS
1	B	124	ASN
1	B	125	LEU
1	B	128	LEU
1	B	151	LEU
1	B	169	LYS
1	B	180	ASN
1	B	197	LEU
1	B	211	ILE
1	B	212	LEU
1	B	219	VAL
1	B	232	ASP
1	B	259	LEU
1	B	276	GLN
1	B	285	LEU
1	B	302	ILE
1	B	304	GLN
1	B	315	LEU
1	B	316	ARG
1	B	319	SER
1	B	321	VAL
1	B	346	GLN
1	B	368	PRO
1	B	417	GLN
1	B	428	LEU
1	B	436	LEU
1	C	16	ILE
1	C	26	GLN
1	C	61	ARG
1	C	91	LEU

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Mol	Chain	Res	Type
1	C	102	LEU
1	C	106	LEU
1	C	125	LEU
1	C	126	LYS
1	C	128	LEU
1	C	145	ILE
1	C	149	PHE
1	C	151	LEU
1	C	156	ASN
1	C	159	SER
1	C	169	LYS
1	C	180	ASN
1	C	212	LEU
1	C	219	VAL
1	C	255	LEU
1	C	259	LEU
1	C	267	GLU
1	C	285	LEU
1	C	300	THR
1	C	301	LYS
1	C	314	LEU
1	C	315	LEU
1	C	325	VAL
1	C	326	GLU
1	C	343	SER
1	C	346	GLN
1	C	348	LEU
1	C	367	SER
1	C	403	LYS
1	C	410	LYS
1	C	419	LYS
1	C	420	LYS
1	C	428	LEU
1	C	436	LEU
1	C	437	LEU
1	D	14	LYS
1	D	16	ILE
1	D	17	MET
1	D	61	ARG
1	D	62	LYS
1	D	65	SER
1	D	66	ILE

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Mol	Chain	Res	Type
1	D	91	LEU
1	D	102	LEU
1	D	106	LEU
1	D	124	ASN
1	D	125	LEU
1	D	128	LEU
1	D	129	VAL
1	D	130	ILE
1	D	157	SER
1	D	169	LYS
1	D	188[A]	ILE
1	D	188[B]	ILE
1	D	205	ILE
1	D	211	ILE
1	D	235	GLN
1	D	243	ILE
1	D	247	LEU
1	D	252	VAL
1	D	257	PRO
1	D	259	LEU
1	D	285	LEU
1	D	288	LEU
1	D	296	GLN
1	D	302	ILE
1	D	310	THR
1	D	313	SER
1	D	316	ARG
1	D	342	LYS
1	D	346	GLN
1	D	348	LEU
1	D	403	LYS
1	D	410	LYS
1	D	419	LYS
1	D	421	LYS
1	D	433	SER
1	D	436	LEU
1	D	437	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN

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Mol	Chain	Res	Type
1	A	31	ASN
1	A	208	ASN
1	A	228	ASN
1	A	276	GLN
1	A	346	GLN
1	A	384	ASN
1	A	417	GLN
1	B	15	ASN
1	B	82	ASN
1	B	158	GLN
1	B	236	GLN
1	B	304	GLN
1	B	344	HIS
1	B	349	GLN
1	C	15	ASN
1	C	22	ASN
1	C	82	ASN
1	C	97	GLN
1	C	180	ASN
1	C	192	ASN
1	C	208	ASN
1	C	228	ASN
1	C	278	ASN
1	C	344	HIS
1	D	82	ASN
1	D	235	GLN
1	D	261	GLN
1	D	278	ASN
1	D	296	GLN
1	D	307	GLN
1	D	346	GLN
1	D	351	ASN

### 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 [i](#)

There are no carbohydrates 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	384/451 (85%)	-0.22	10 (2%) 59 68	31, 46, 76, 117	0
1	B	388/451 (86%)	-0.13	9 (2%) 64 72	31, 48, 78, 133	0
1	C	388/451 (86%)	0.07	27 (6%) 19 26	32, 53, 96, 112	0
1	D	383/451 (84%)	-0.09	9 (2%) 64 72	34, 51, 79, 117	0
All	All	1543/1804 (85%)	-0.09	55 (3%) 46 57	31, 49, 87, 133	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	LEU	6.9
1	B	61	ARG	5.8
1	A	61	ARG	5.6
1	C	31	ASN	5.5
1	D	211	ILE	5.3
1	C	29	LEU	5.2
1	D	28	TYR	5.1
1	B	29	LEU	5.0
1	B	28	TYR	4.9
1	D	61	ARG	4.9
1	C	60	GLY	4.8
1	A	212	LEU	4.7
1	A	31	ASN	4.6
1	C	312	ILE	4.4
1	C	155	GLY	4.4
1	B	212	LEU	4.3
1	B	211	ILE	4.3
1	C	212	LEU	4.0
1	C	299	ASP	4.0
1	C	30	PRO	4.0
1	D	30	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	219	VAL	3.6
1	C	61	ARG	3.5
1	C	156	ASN	3.5
1	A	6	MET	3.4
1	B	30	PRO	3.4
1	C	6	MET	3.4
1	C	315	LEU	3.4
1	A	151	LEU	3.2
1	D	219	VAL	3.0
1	D	62	LYS	2.9
1	B	62	LYS	2.7
1	D	64	GLU	2.7
1	C	419	LYS	2.7
1	A	29	LEU	2.7
1	C	317	VAL	2.6
1	C	314	LEU	2.6
1	C	28	TYR	2.6
1	C	63	PHE	2.6
1	C	62	LYS	2.6
1	D	151	LEU	2.6
1	C	322	LYS	2.5
1	A	351	ASN	2.4
1	C	268	ASP	2.4
1	C	300	THR	2.3
1	C	318	GLY	2.3
1	A	419	LYS	2.3
1	B	64	GLU	2.2
1	A	30	PRO	2.2
1	C	319	SER	2.2
1	C	219	VAL	2.2
1	A	315	LEU	2.1
1	C	7	PRO	2.1
1	C	246	GLY	2.1
1	C	64	GLU	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 carbohydrates 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.