



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:54 AM GMT

PDB ID : 3CKY  
Title : Structural and Kinetic Properties of a beta-hydroxyacid dehydrogenase involved in nicotinate fermentation  
Authors : Reitz, S.; Alhapel, A.; Pierik, A.J.; Essen, L.-O.  
Deposited on : 2008-03-18  
Resolution : 2.30 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

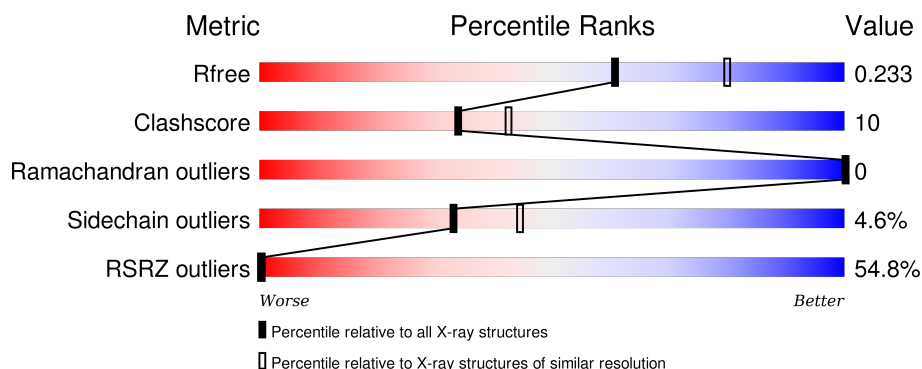
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	301	<div> <div>55%</div> <div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	301	<div> <div>36%</div> <div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	301	<div> <div>67%</div> <div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	301	<div> <div>48%</div> <div> <div>67%</div> <div>11%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8515 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-hydroxymethyl glutarate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	3	1	0
			2117	1333	349	412	23			
1	B	296	Total	C	N	O	S	6	1	0
			2113	1331	348	411	23			
1	C	296	Total	C	N	O	S	14	1	0
			2111	1330	348	410	23			
1	D	240	Total	C	N	O	S	0	2	0
			1727	1089	282	338	18			

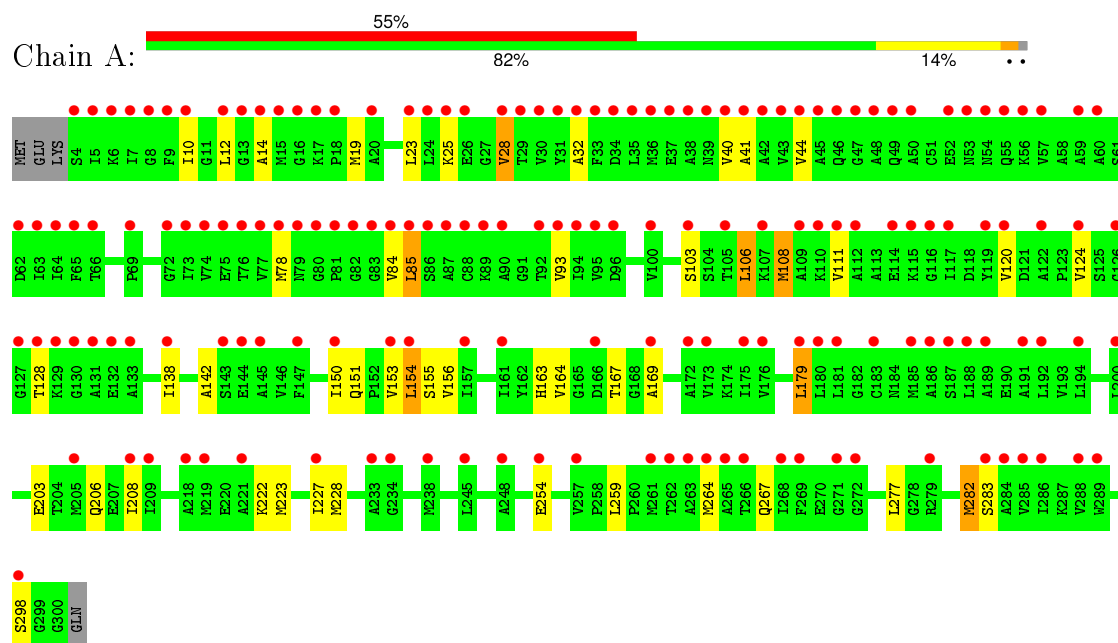
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	158	Total	O	0	0
			158	158		
2	C	96	Total	O	0	0
			96	96		
2	D	70	Total	O	0	0
			70	70		

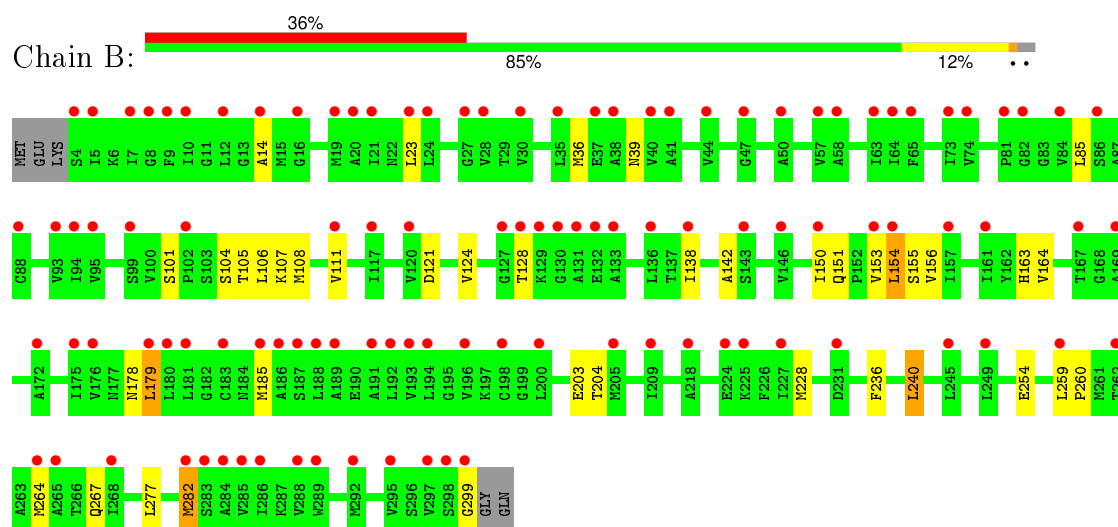
### 3 Residue-property plots

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.

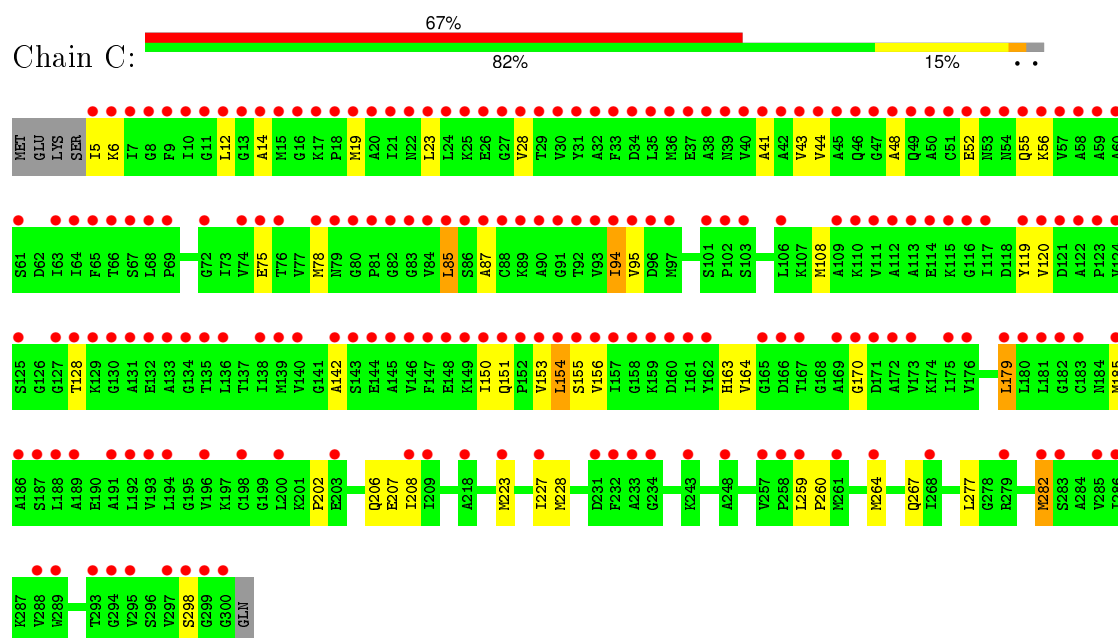
- Molecule 1: 2-hydroxymethyl glutarate dehydrogenase



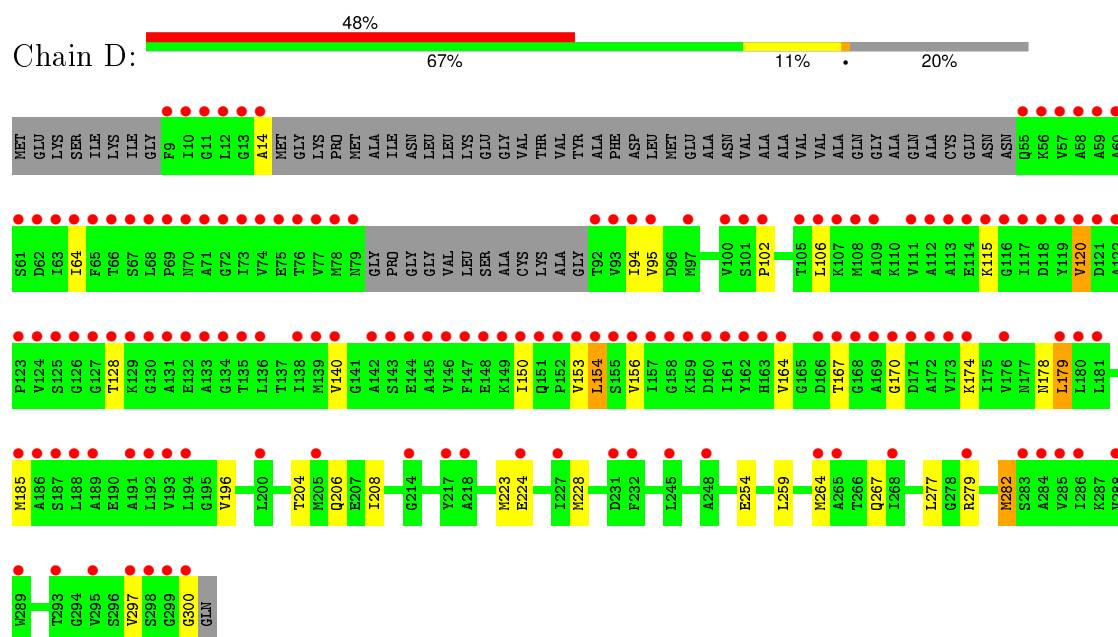
- Molecule 1: 2-hydroxymethyl glutarate dehydrogenase



- Molecule 1: 2-hydroxymethyl glutarate dehydrogenase



- Molecule 1: 2-hydroxymethyl glutarate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.98Å 175.78Å 83.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.47 – 2.30 24.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (24.47-2.30) 95.2 (24.47-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.222 0.203 , 0.233	Depositor DCC
$R_{free}$ test set	2674 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.3	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 52485 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	0.45	0/2144	0.53	1/2888 (0.0%)
1	B	0.51	0/2140	0.57	1/2883 (0.0%)
1	C	0.45	0/2138	0.54	1/2880 (0.0%)
1	D	0.45	0/1751	0.54	1/2354 (0.0%)
All	All	0.47	0/8173	0.54	4/11005 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	179	LEU	CA-CB-CG	5.76	128.56	115.30
1	D	179	LEU	CA-CB-CG	5.67	128.35	115.30
1	C	179	LEU	CA-CB-CG	5.33	127.56	115.30

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	2117	0	2174	60	0
1	B	2113	0	2171	46	0
1	C	2111	0	2169	55	0
1	D	1727	0	1772	43	0
2	A	123	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	158	0	0	3	0
2	C	96	0	0	0	0
2	D	70	0	0	2	0
All	All	8515	0	8286	165	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 (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264[A]:MET:CE	1:B:264[A]:MET:HE3	1.45	1.46
1:C:264[B]:MET:HE1	1:D:264[B]:MET:SD	1.83	1.16
1:C:264[B]:MET:CE	1:D:264[B]:MET:HE1	1.76	1.14
1:A:264[A]:MET:SD	1:B:264[A]:MET:HE3	1.89	1.13
1:C:264[B]:MET:HE2	1:D:264[B]:MET:CE	1.81	1.10
1:B:236:PHE:CE1	1:B:240:LEU:HD13	1.87	1.10
1:C:264[B]:MET:HE2	1:D:264[B]:MET:HE1	1.09	1.08
1:A:264[A]:MET:HE2	1:B:264[A]:MET:HE3	1.25	1.07
1:C:264[B]:MET:CE	1:D:264[B]:MET:CE	2.31	1.07
1:A:264[A]:MET:SD	1:B:264[A]:MET:CE	2.43	1.06
1:C:264[B]:MET:CE	1:D:264[B]:MET:SD	2.42	1.06
1:A:264[A]:MET:CE	1:B:264[A]:MET:CE	2.35	1.04
1:B:236:PHE:HE1	1:B:240:LEU:HD13	1.29	0.94
1:C:78:MET:CE	1:C:85:LEU:HD13	1.99	0.93
1:B:153:VAL:O	1:B:156:VAL:HG12	1.74	0.86
1:A:153:VAL:O	1:A:156:VAL:HG12	1.78	0.82
1:A:23:LEU:HD23	1:A:156:VAL:HG11	1.62	0.81
1:A:10:ILE:HD13	1:A:84:VAL:HG21	1.63	0.80
1:C:264[B]:MET:SD	1:D:264[B]:MET:CE	2.69	0.80
1:C:153:VAL:O	1:C:156:VAL:HG12	1.81	0.80
1:A:264[A]:MET:SD	1:B:264[A]:MET:HE2	2.22	0.79
1:B:264[B]:MET:HG3	1:C:264[B]:MET:HG3	1.65	0.79
1:D:185:MET:HG2	1:D:282:MET:HE3	1.65	0.79
1:D:153:VAL:O	1:D:156:VAL:HG12	1.83	0.79
1:B:23:LEU:HD23	1:B:156:VAL:HG11	1.65	0.77
1:A:264[B]:MET:HE3	1:B:264[B]:MET:SD	2.25	0.77
1:C:185:MET:HG2	1:C:282:MET:HE3	1.67	0.76
1:C:23:LEU:HD23	1:C:156:VAL:HG11	1.67	0.76
1:A:78:MET:CE	1:A:85:LEU:HD13	2.16	0.75
1:C:78:MET:HE3	1:C:85:LEU:HD13	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:O	1:A:44:VAL:HG13	1.89	0.72
1:A:78:MET:HE3	1:A:85:LEU:HD13	1.72	0.72
1:D:102:PRO:O	1:D:106:LEU:HD13	1.91	0.70
1:B:185:MET:HG2	1:B:282:MET:HE3	1.74	0.70
1:C:264[B]:MET:SD	1:D:264[B]:MET:HE1	2.29	0.69
1:D:224:GLU:HA	1:D:228:MET:CE	2.24	0.67
1:A:264[A]:MET:HE1	1:B:264[A]:MET:HE3	1.67	0.65
1:A:208:ILE:HD11	1:D:164:VAL:HG12	1.79	0.65
1:A:208:ILE:CD1	1:D:164:VAL:HG12	2.26	0.65
1:C:12:LEU:HD21	1:C:43:VAL:CG1	2.27	0.65
1:D:224:GLU:HA	1:D:228:MET:HE2	1.77	0.65
1:A:259:LEU:H	1:C:267:GLN:NE2	1.94	0.64
1:C:206:GLN:HB2	1:C:228:MET:HE1	1.80	0.63
1:D:254:GLU:OE1	2:D:359:HOH:O	2.16	0.62
1:B:23:LEU:CD2	1:B:156:VAL:HG11	2.30	0.61
1:A:41:ALA:HA	1:A:44:VAL:HG22	1.80	0.61
1:C:264[B]:MET:SD	1:D:264[B]:MET:HE3	2.41	0.61
1:C:41:ALA:HA	1:C:44:VAL:HG12	1.83	0.60
1:A:23:LEU:CD2	1:A:156:VAL:HG11	2.30	0.60
1:D:164:VAL:HG21	1:D:170:GLY:HA2	1.83	0.60
1:C:185:MET:HG2	1:C:282:MET:CE	2.31	0.60
1:D:185:MET:HG2	1:D:282:MET:CE	2.32	0.59
1:A:264[A]:MET:HE2	1:B:264[A]:MET:CE	2.17	0.59
1:C:78:MET:HE2	1:C:85:LEU:HD13	1.83	0.59
1:C:12:LEU:HD21	1:C:43:VAL:HG13	1.84	0.59
1:C:164:VAL:HG21	1:C:170:GLY:HA2	1.84	0.59
1:A:222:LYS:HG3	1:A:282:MET:HE1	1.84	0.59
1:B:254:GLU:OE1	2:B:306:HOH:O	2.17	0.59
1:C:78:MET:CE	1:C:85:LEU:CD1	2.80	0.58
1:B:153:VAL:O	1:B:156:VAL:CG1	2.47	0.58
1:C:94:ILE:HG21	1:C:119:TYR:CD1	2.39	0.58
1:A:264[A]:MET:HE1	1:B:264[A]:MET:CE	2.28	0.57
1:B:36:MET:HE3	1:B:39:ASN:HD21	1.69	0.57
1:C:264[B]:MET:HE2	1:D:264[B]:MET:SD	2.29	0.57
1:C:23:LEU:CD2	1:C:156:VAL:HG11	2.33	0.57
1:A:254:GLU:OE1	2:A:355:HOH:O	2.17	0.56
1:A:78:MET:HE2	1:A:85:LEU:HD13	1.87	0.56
1:A:264[A]:MET:HG3	1:B:264[A]:MET:CE	2.35	0.56
1:C:94:ILE:HG23	1:C:119:TYR:HA	1.88	0.56
1:C:206:GLN:HB2	1:C:223:MET:HE2	1.88	0.55
1:B:267:GLN:NE2	1:D:259:LEU:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264[A]:MET:CG	1:B:264[A]:MET:CE	2.85	0.55
1:D:206:GLN:HG3	1:D:223:MET:HG2	1.90	0.54
1:C:206:GLN:HG3	1:C:223:MET:HG2	1.89	0.54
1:A:259:LEU:H	1:C:267:GLN:HE21	1.55	0.54
1:A:108:MET:HA	1:A:108:MET:HE2	1.90	0.54
1:A:264[A]:MET:CG	1:B:264[A]:MET:HE3	2.38	0.52
1:C:202:PRO:C	1:C:228:MET:HE2	2.29	0.52
1:D:174:LYS:HD2	1:D:178:ASN:HD21	1.74	0.52
1:A:106:LEU:HD13	1:A:167:THR:HG22	1.91	0.52
1:C:23:LEU:HB3	1:C:28:VAL:CG2	2.40	0.52
1:C:94:ILE:CG2	1:C:119:TYR:CD1	2.93	0.51
1:C:55:GLN:HG3	1:C:87:ALA:HB2	1.92	0.51
1:B:151:GLN:NE2	1:B:155:SER:OG	2.43	0.50
1:B:142:ALA:O	1:B:163:HIS:HE1	1.95	0.50
1:D:204:THR:O	1:D:208:ILE:HD13	2.11	0.50
1:A:153:VAL:O	1:A:156:VAL:CG1	2.56	0.50
1:C:153:VAL:O	1:C:156:VAL:CG1	2.57	0.49
1:B:259:LEU:H	1:D:267:GLN:NE2	2.10	0.49
1:B:14:ALA:HB1	1:B:128:THR:HG21	1.93	0.49
1:C:14:ALA:HB1	1:C:128:THR:HG21	1.94	0.49
1:B:236:PHE:CE1	1:B:240:LEU:CD1	2.79	0.49
1:D:185:MET:CG	1:D:282:MET:HE3	2.40	0.49
1:C:12:LEU:HD21	1:C:43:VAL:HG11	1.95	0.49
1:A:203:GLU:HG3	1:A:228:MET:HE3	1.96	0.48
1:A:10:ILE:CD1	1:A:84:VAL:HG21	2.41	0.48
1:C:151:GLN:NE2	1:C:155:SER:OG	2.47	0.48
1:D:224:GLU:HA	1:D:228:MET:HE3	1.95	0.48
1:C:41:ALA:O	1:C:44:VAL:HG12	2.14	0.48
1:A:78:MET:CE	1:A:85:LEU:CD1	2.90	0.48
1:A:206:GLN:HG3	1:A:223:MET:HG2	1.95	0.48
1:C:14:ALA:HB1	1:C:128:THR:CG2	2.44	0.47
1:A:23:LEU:O	1:A:28:VAL:HG13	2.14	0.47
1:B:185:MET:HG2	1:B:282:MET:CE	2.43	0.47
1:D:224:GLU:CA	1:D:228:MET:HE2	2.44	0.47
1:D:300:GLY:HA2	2:D:362:HOH:O	2.14	0.47
1:A:14:ALA:HB1	1:A:128:THR:HG21	1.96	0.47
1:C:44:VAL:HG23	1:C:48:ALA:O	2.15	0.47
1:D:196:VAL:HG21	1:D:297:VAL:HG22	1.97	0.46
1:A:267:GLN:NE2	1:C:259:LEU:H	2.13	0.46
1:A:222:LYS:HE3	1:A:282:MET:CE	2.45	0.46
1:D:64:ILE:HD12	1:D:94:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264[A]:MET:HG3	1:B:264[A]:MET:HE1	1.97	0.45
1:C:19:MET:HB2	1:C:19:MET:HE2	1.82	0.45
1:C:78:MET:HE2	1:C:85:LEU:CD1	2.44	0.45
1:A:103:SER:HG	1:A:254:GLU:CD	2.19	0.45
1:B:14:ALA:HB1	1:B:128:THR:CG2	2.46	0.45
1:D:150:ILE:HG13	1:D:154:LEU:HD22	1.98	0.45
1:A:264[A]:MET:HE1	1:C:260:PRO:CB	2.47	0.45
1:D:174:LYS:HD2	1:D:178:ASN:ND2	2.31	0.45
1:B:260:PRO:HB3	1:D:264[A]:MET:HE1	1.99	0.45
1:A:108:MET:O	1:A:111:VAL:HG22	2.16	0.45
1:B:299:GLY:C	2:B:450:HOH:O	2.55	0.45
1:A:282:MET:HE3	1:A:283:SER:N	2.32	0.45
1:A:151:GLN:NE2	1:A:155:SER:OG	2.50	0.44
1:A:14:ALA:HB1	1:A:128:THR:CG2	2.47	0.44
1:D:106:LEU:HD12	1:D:167:THR:HG22	1.99	0.44
1:B:105:THR:HG21	1:B:121:ASP:HB3	2.00	0.44
1:A:164:VAL:HG23	1:A:169:ALA:CB	2.48	0.44
1:B:259:LEU:H	1:D:267:GLN:HE21	1.66	0.44
1:A:12:LEU:HD11	1:A:32:ALA:HB1	1.99	0.44
1:D:14:ALA:HB1	1:D:128:THR:HG21	1.99	0.44
1:C:142:ALA:O	1:C:163:HIS:HE1	2.00	0.44
1:A:19:MET:HB2	1:A:19:MET:HE2	1.85	0.44
1:B:264[B]:MET:CG	1:C:264[B]:MET:HG3	2.43	0.43
1:A:41:ALA:O	1:A:44:VAL:HG22	2.19	0.43
1:A:108:MET:HA	1:A:108:MET:CE	2.47	0.43
1:C:150:ILE:HG13	1:C:154:LEU:HD22	2.00	0.43
1:B:108:MET:O	1:B:111:VAL:HG22	2.18	0.43
1:A:78:MET:HE2	1:A:85:LEU:CD1	2.48	0.43
1:B:178:ASN:HB3	2:B:311:HOH:O	2.18	0.43
1:C:185:MET:CG	1:C:282:MET:HE3	2.44	0.43
1:A:142:ALA:O	1:A:163:HIS:HE1	2.02	0.43
1:B:264[B]:MET:SD	1:D:264[B]:MET:HE2	2.59	0.43
1:B:150:ILE:HG13	1:B:154:LEU:HD22	2.01	0.43
1:C:227:ILE:O	1:C:298:SER:HA	2.18	0.43
1:C:94:ILE:HD12	1:C:95:VAL:N	2.34	0.42
1:A:106:LEU:HD13	1:A:167:THR:CG2	2.49	0.42
1:C:23:LEU:HB3	1:C:28:VAL:HG21	2.01	0.42
1:D:208:ILE:N	1:D:208:ILE:HD12	2.34	0.42
1:A:227:ILE:O	1:A:298:SER:HA	2.20	0.42
1:B:124:VAL:HG12	1:B:138:ILE:HG12	2.00	0.42
1:A:150:ILE:HG13	1:A:154:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:HG12	1:C:208:ILE:HD11	2.01	0.42
1:D:95:VAL:HA	1:D:120:VAL:HG22	2.02	0.42
1:A:282:MET:CE	1:A:283:SER:N	2.83	0.42
1:D:14:ALA:HB1	1:D:128:THR:CG2	2.49	0.42
1:C:55:GLN:CG	1:C:87:ALA:HB2	2.50	0.42
1:A:124:VAL:HG12	1:A:138:ILE:HG12	2.02	0.41
1:A:93:VAL:HG11	1:A:150:ILE:HG21	2.02	0.41
1:B:203:GLU:HG3	1:B:228:MET:HE3	2.03	0.40
1:D:140:VAL:O	1:D:164:VAL:HG22	2.21	0.40
1:B:267:GLN:HE21	1:D:259:LEU:H	1.69	0.40
1:A:25:LYS:HB2	1:A:25:LYS:HZ2	1.86	0.40
1:B:101:SER:O	1:B:104:SER:HB3	2.20	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	296/301 (98%)	294 (99%)	2 (1%)	0	100	100
1	B	295/301 (98%)	293 (99%)	2 (1%)	0	100	100
1	C	295/301 (98%)	290 (98%)	5 (2%)	0	100	100
1	D	236/301 (78%)	230 (98%)	6 (2%)	0	100	100
All	All	1122/1204 (93%)	1107 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	221/224 (99%)	212 (96%)	9 (4%)	37	50
1	B	221/224 (99%)	212 (96%)	9 (4%)	37	50
1	C	220/224 (98%)	206 (94%)	14 (6%)	22	28
1	D	183/224 (82%)	176 (96%)	7 (4%)	40	54
All	All	845/896 (94%)	806 (95%)	39 (5%)	33	44

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	85	LEU
1	A	106	LEU
1	A	108	MET
1	A	120	VAL
1	A	154	LEU
1	A	179	LEU
1	A	277	LEU
1	A	282	MET
1	B	85	LEU
1	B	106	LEU
1	B	107	LYS
1	B	154	LEU
1	B	179	LEU
1	B	204	THR
1	B	240	LEU
1	B	277	LEU
1	B	282	MET
1	C	5	ILE
1	C	6	LYS
1	C	52	GLU
1	C	56	LYS
1	C	75	GLU
1	C	85	LEU
1	C	94	ILE
1	C	108	MET
1	C	120	VAL
1	C	154	LEU

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Mol	Chain	Res	Type
1	C	179	LEU
1	C	207	GLU
1	C	277	LEU
1	C	282	MET
1	D	115	LYS
1	D	120	VAL
1	D	154	LEU
1	D	179	LEU
1	D	277	LEU
1	D	279	ARG
1	D	282	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	79	ASN
1	A	151	GLN
1	A	163	HIS
1	A	241	GLN
1	A	256	ASN
1	A	267	GLN
1	B	39	ASN
1	B	79	ASN
1	B	151	GLN
1	B	163	HIS
1	B	242	HIS
1	B	256	ASN
1	B	267	GLN
1	C	79	ASN
1	C	151	GLN
1	C	163	HIS
1	C	256	ASN
1	C	267	GLN
1	D	79	ASN
1	D	151	GLN
1	D	163	HIS
1	D	256	ASN
1	D	267	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 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	297/301 (98%)	2.64	165 (55%) <b>0</b> <b>0</b>	38, 62, 75, 77	1 (0%)
1	B	296/301 (98%)	1.82	108 (36%) <b>0</b> <b>0</b>	38, 62, 74, 77	2 (0%)
1	C	296/301 (98%)	3.68	201 (67%) <b>0</b> <b>0</b>	38, 62, 74, 77	4 (1%)
1	D	240/301 (79%)	3.22	145 (60%) <b>0</b> <b>0</b>	26, 47, 68, 76	0
All	All	1129/1204 (93%)	2.82	619 (54%) <b>0</b> <b>0</b>	26, 61, 74, 77	7 (0%)

All (619) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	SER	14.6
1	A	81	PRO	13.9
1	C	35	LEU	13.9
1	D	156	VAL	12.4
1	D	111	VAL	12.2
1	C	29	THR	12.2
1	C	130	GLY	12.0
1	D	117	ILE	11.7
1	C	59	ALA	11.6
1	C	36	MET	11.5
1	C	300	GLY	11.4
1	C	39	ASN	11.2
1	D	57	VAL	10.4
1	C	14	ALA	10.4
1	C	41	ALA	10.3
1	C	5	ILE	10.1
1	C	28	VAL	9.9
1	C	25	LYS	9.9
1	A	64	ILE	9.8
1	C	81	PRO	9.5
1	D	131	ALA	9.4

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Mol	Chain	Res	Type	RSRZ
1	C	45	ALA	9.2
1	A	82	GLY	9.0
1	D	59	ALA	8.9
1	C	166	ASP	8.8
1	C	60	ALA	8.8
1	D	13	GLY	8.7
1	A	65	PHE	8.7
1	C	49	GLN	8.7
1	C	117	ILE	8.6
1	C	142	ALA	8.6
1	C	61	SER	8.5
1	D	135	THR	8.5
1	D	300	GLY	8.5
1	C	40	VAL	8.4
1	C	113	ALA	8.4
1	A	80	GLY	8.3
1	C	131	ALA	8.3
1	D	60	ALA	8.2
1	A	41	ALA	8.2
1	D	113	ALA	8.2
1	C	299	GLY	8.2
1	D	127	GLY	8.2
1	C	147	PHE	8.1
1	C	48	ALA	8.1
1	C	24	LEU	8.1
1	C	18	PRO	8.0
1	D	12	LEU	8.0
1	C	135	THR	8.0
1	D	152	PRO	7.9
1	C	30	VAL	7.8
1	D	69	PRO	7.8
1	A	84	VAL	7.7
1	A	43	VAL	7.7
1	A	4	SER	7.6
1	D	92	THR	7.6
1	C	8	GLY	7.6
1	C	42	ALA	7.5
1	C	150	ILE	7.5
1	C	65	PHE	7.4
1	C	157	ILE	7.4
1	C	133	ALA	7.3
1	C	23	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	D	14	ALA	7.3
1	D	130	GLY	7.3
1	D	146	VAL	7.2
1	C	33	PHE	7.2
1	C	132	GLU	7.1
1	C	21	ILE	7.0
1	D	158	GLY	7.0
1	A	112	ALA	7.0
1	A	9	PHE	6.9
1	C	127	GLY	6.9
1	C	64	ILE	6.9
1	D	142	ALA	6.8
1	B	4	SER	6.8
1	D	126	GLY	6.8
1	D	129	LYS	6.8
1	C	87	ALA	6.7
1	D	148	GLU	6.7
1	A	95	VAL	6.6
1	C	95	VAL	6.6
1	C	112	ALA	6.6
1	D	132	GLU	6.6
1	A	116	GLY	6.5
1	C	111	VAL	6.5
1	C	80	GLY	6.5
1	C	129	LYS	6.5
1	A	44	VAL	6.5
1	C	72	GLY	6.5
1	D	157	ILE	6.4
1	A	129	LYS	6.4
1	C	7	ILE	6.4
1	D	150	ILE	6.3
1	B	64	ILE	6.3
1	D	10	ILE	6.3
1	A	37	GLU	6.3
1	D	78	MET	6.3
1	C	298	SER	6.2
1	A	133	ALA	6.1
1	A	111	VAL	6.1
1	A	35	LEU	6.1
1	C	50	ALA	6.1
1	A	50	ALA	6.0
1	A	36	MET	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	160	ASP	6.0
1	D	68	LEU	6.0
1	C	152	PRO	6.0
1	A	6	LYS	6.0
1	C	9	PHE	5.9
1	D	128	THR	5.9
1	D	62	ASP	5.9
1	C	122	ALA	5.9
1	C	176	VAL	5.9
1	C	66	THR	5.9
1	B	81	PRO	5.8
1	C	167	THR	5.8
1	D	116	GLY	5.8
1	D	299	GLY	5.8
1	C	153	VAL	5.8
1	C	16	GLY	5.7
1	C	43	VAL	5.7
1	D	72	GLY	5.7
1	B	95	VAL	5.7
1	C	82	GLY	5.6
1	A	94	ILE	5.6
1	A	66	THR	5.6
1	D	74	VAL	5.6
1	A	24	LEU	5.6
1	B	299	GLY	5.6
1	D	159	LYS	5.6
1	C	116	GLY	5.5
1	A	63	ILE	5.5
1	C	154	LEU	5.5
1	D	64	ILE	5.5
1	D	63	ILE	5.5
1	A	40	VAL	5.5
1	C	6	LYS	5.4
1	D	153	VAL	5.4
1	C	34	ASP	5.4
1	C	115	LYS	5.4
1	C	90	ALA	5.4
1	D	143	SER	5.4
1	B	94	ILE	5.4
1	A	72	GLY	5.4
1	C	38	ALA	5.4
1	D	154	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	159	LYS	5.3
1	D	134	GLY	5.3
1	D	155	SER	5.3
1	D	160	ASP	5.3
1	C	57	VAL	5.3
1	C	140	VAL	5.3
1	C	89	LYS	5.3
1	C	44	VAL	5.2
1	B	65	PHE	5.2
1	C	293	THR	5.2
1	B	191	ALA	5.2
1	C	22	ASN	5.1
1	A	128	THR	5.1
1	D	73	ILE	5.1
1	B	50	ALA	5.1
1	D	58	ALA	5.1
1	A	42	ALA	5.1
1	D	133	ALA	5.0
1	A	31	TYR	5.0
1	A	130	GLY	5.0
1	A	14	ALA	5.0
1	C	27	GLY	5.0
1	C	156	VAL	5.0
1	C	123	PRO	5.0
1	D	95	VAL	4.9
1	C	56	LYS	4.8
1	B	169	ALA	4.8
1	D	192	LEU	4.8
1	A	103	SER	4.8
1	C	128	THR	4.8
1	C	148	GLU	4.8
1	C	84	VAL	4.8
1	C	145	ALA	4.7
1	B	35	LEU	4.7
1	D	298	SER	4.7
1	D	167	THR	4.7
1	D	123	PRO	4.7
1	A	38	ALA	4.7
1	D	145	ALA	4.7
1	A	49	GLN	4.7
1	C	169	ALA	4.7
1	A	285	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	52	GLU	4.7
1	C	136	LEU	4.6
1	C	151	GLN	4.6
1	C	146	VAL	4.6
1	C	185	MET	4.6
1	C	189	ALA	4.6
1	C	10	ILE	4.6
1	A	86	SER	4.6
1	D	114	GLU	4.6
1	C	85	LEU	4.6
1	B	128	THR	4.5
1	C	12	LEU	4.5
1	A	28	VAL	4.5
1	A	176	VAL	4.5
1	A	288	VAL	4.5
1	A	83	GLY	4.5
1	D	122	ALA	4.4
1	A	145	ALA	4.4
1	D	77	VAL	4.4
1	A	179	LEU	4.4
1	C	192	LEU	4.4
1	A	45	ALA	4.4
1	D	115	LYS	4.4
1	C	170	GLY	4.4
1	D	285	VAL	4.3
1	A	286	ILE	4.3
1	C	158	GLY	4.3
1	A	93	VAL	4.3
1	C	32	ALA	4.3
1	A	117	ILE	4.3
1	C	233	ALA	4.3
1	C	91	GLY	4.3
1	C	149	LYS	4.2
1	A	85	LEU	4.2
1	C	124	VAL	4.2
1	A	87	ALA	4.2
1	A	143	SER	4.2
1	D	191	ALA	4.2
1	C	297	VAL	4.2
1	C	88	CYS	4.2
1	C	31	TYR	4.1
1	A	105	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	298	SER	4.1
1	A	56	LYS	4.1
1	D	106	LEU	4.1
1	D	56	LYS	4.1
1	B	120	VAL	4.1
1	D	108	MET	4.1
1	D	169	ALA	4.1
1	A	23	LEU	4.1
1	C	63	ILE	4.1
1	A	53	ASN	4.1
1	A	234	GLY	4.1
1	B	288	VAL	4.0
1	A	8	GLY	4.0
1	A	32	ALA	4.0
1	D	289	TRP	4.0
1	A	144	GLU	4.0
1	C	51	CYS	4.0
1	A	90	ALA	4.0
1	C	119	TYR	4.0
1	A	180	LEU	4.0
1	C	68	LEU	4.0
1	C	78	MET	4.0
1	B	193	VAL	3.9
1	C	161	ILE	4.0
1	D	9	PHE	3.9
1	C	144	GLU	3.9
1	D	66	THR	3.9
1	A	298	SER	3.9
1	D	125	SER	3.9
1	C	188	LEU	3.9
1	B	63	ILE	3.9
1	A	5	ILE	3.9
1	D	105	THR	3.9
1	B	180	LEU	3.9
1	C	19	MET	3.8
1	A	284	ALA	3.8
1	C	138	ILE	3.8
1	C	37	GLU	3.8
1	A	79	ASN	3.8
1	D	185	MET	3.8
1	B	5	ILE	3.8
1	D	193	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	76	THR	3.8
1	C	139	MET	3.8
1	A	110	LYS	3.7
1	D	144	GLU	3.7
1	A	127	GLY	3.7
1	D	171	ASP	3.7
1	C	162	TYR	3.7
1	D	107	LYS	3.7
1	B	189	ALA	3.7
1	A	34	ASP	3.7
1	D	112	ALA	3.7
1	A	88	CYS	3.7
1	A	107	LYS	3.7
1	C	15	MET	3.7
1	A	52	GLU	3.7
1	D	100	VAL	3.7
1	A	59	ALA	3.7
1	B	9	PHE	3.7
1	C	268	ILE	3.6
1	B	188	LEU	3.6
1	D	11	GLY	3.6
1	B	179	LEU	3.6
1	C	200	LEU	3.6
1	C	286	ILE	3.6
1	C	288	VAL	3.6
1	D	173	VAL	3.6
1	D	189	ALA	3.6
1	D	55	GLN	3.6
1	A	13	GLY	3.6
1	A	119	TYR	3.6
1	B	192	LEU	3.6
1	C	92	THR	3.5
1	B	86	SER	3.5
1	C	109	ALA	3.5
1	C	120	VAL	3.5
1	A	46	GLN	3.5
1	C	86	SER	3.5
1	A	10	ILE	3.5
1	C	180	LEU	3.5
1	D	181	LEU	3.5
1	A	33	PHE	3.5
1	A	29	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	150	ILE	3.5
1	D	186	ALA	3.5
1	D	151	GLN	3.4
1	A	20	ALA	3.4
1	D	162	TYR	3.4
1	D	286	ILE	3.4
1	C	55	GLN	3.4
1	D	194	LEU	3.4
1	D	279	ARG	3.4
1	A	138	ILE	3.4
1	D	138	ILE	3.4
1	D	188	LEU	3.4
1	A	131	ALA	3.4
1	C	172	ALA	3.4
1	C	69	PRO	3.4
1	A	268	ILE	3.3
1	C	194	LEU	3.3
1	C	191	ALA	3.3
1	A	186	ALA	3.3
1	B	268	ILE	3.3
1	B	82	GLY	3.3
1	C	294	GLY	3.3
1	A	150	ILE	3.2
1	B	133	ALA	3.2
1	B	172	ALA	3.2
1	B	24	LEU	3.2
1	D	124	VAL	3.2
1	D	297	VAL	3.2
1	D	149	LYS	3.2
1	B	186	ALA	3.2
1	C	186	ALA	3.2
1	A	191	ALA	3.2
1	C	181	LEU	3.2
1	A	39	ASN	3.2
1	C	193	VAL	3.2
1	D	93	VAL	3.2
1	D	283	SER	3.2
1	C	94	ILE	3.1
1	B	132	GLU	3.1
1	A	47	GLY	3.1
1	D	268	ILE	3.1
1	D	163	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	176	VAL	3.1
1	A	92	THR	3.1
1	B	117	ILE	3.1
1	B	154	LEU	3.1
1	A	15	MET	3.1
1	B	194	LEU	3.1
1	D	136	LEU	3.1
1	B	57	VAL	3.1
1	C	227	ILE	3.1
1	A	124	VAL	3.1
1	B	93	VAL	3.1
1	A	7	ILE	3.0
1	A	264[A]	MET	3.0
1	A	173	VAL	3.0
1	A	114	GLU	3.0
1	B	286	ILE	3.0
1	B	185	MET	3.0
1	D	180	LEU	3.0
1	B	129	LYS	3.0
1	C	17	LYS	3.0
1	C	295	VAL	3.0
1	B	14	ALA	3.0
1	A	227	ILE	3.0
1	A	166	ASP	3.0
1	D	139	MET	3.0
1	B	289	TRP	3.0
1	A	18	PRO	3.0
1	B	227	ILE	3.0
1	A	200	LEU	3.0
1	C	155	SER	3.0
1	A	271	GLY	3.0
1	A	279	ARG	2.9
1	B	23	LEU	2.9
1	B	259	LEU	2.9
1	D	200	LEU	2.9
1	C	67	SER	2.9
1	B	84	VAL	2.9
1	D	65	PHE	2.9
1	A	126	GLY	2.9
1	B	27	GLY	2.9
1	B	47	GLY	2.9
1	C	114	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	172	ALA	2.9
1	D	284	ALA	2.9
1	A	120	VAL	2.9
1	B	209	ILE	2.9
1	C	231	ASP	2.9
1	C	93	VAL	2.8
1	A	175	ILE	2.8
1	B	58	ALA	2.8
1	A	272	GLY	2.8
1	A	78	MET	2.8
1	A	188	LEU	2.8
1	C	179	LEU	2.8
1	C	46	GLN	2.8
1	A	26	GLU	2.8
1	C	26	GLU	2.8
1	D	224	GLU	2.8
1	B	138	ILE	2.8
1	A	169	ALA	2.8
1	D	102	PRO	2.8
1	B	146	VAL	2.8
1	A	73	ILE	2.8
1	D	170	GLY	2.8
1	A	25	LYS	2.8
1	C	53	ASN	2.8
1	A	181	LEU	2.7
1	D	94	ILE	2.7
1	C	173	VAL	2.7
1	D	288	VAL	2.7
1	A	194	LEU	2.7
1	A	122	ALA	2.7
1	D	109	ALA	2.7
1	C	121	ASP	2.7
1	D	76	THR	2.7
1	A	30	VAL	2.7
1	A	57	VAL	2.7
1	C	264[A]	MET	2.7
1	D	232	PHE	2.7
1	B	283	SER	2.7
1	B	30	VAL	2.7
1	C	258	PRO	2.7
1	D	205	MET	2.7
1	B	175	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	187	SER	2.7
1	C	110	LYS	2.7
1	A	16	GLY	2.7
1	C	76	THR	2.7
1	C	165	GLY	2.7
1	C	75	GLU	2.7
1	D	140	VAL	2.7
1	A	54	ASN	2.6
1	C	261	MET	2.6
1	C	218	ALA	2.6
1	B	262	THR	2.6
1	D	217	TYR	2.6
1	D	120	VAL	2.6
1	A	132	GLU	2.6
1	B	19	MET	2.6
1	B	264[A]	MET	2.6
1	D	97	MET	2.6
1	A	218	ALA	2.6
1	A	62	ASP	2.6
1	C	58	ALA	2.6
1	C	257	VAL	2.6
1	C	143	SER	2.6
1	D	176	VAL	2.6
1	A	262	THR	2.6
1	B	73	ILE	2.6
1	D	147	PHE	2.6
1	D	119	TYR	2.6
1	C	20	ALA	2.6
1	A	238	MET	2.6
1	A	266	THR	2.6
1	B	74	VAL	2.6
1	B	10	ILE	2.6
1	A	254	GLU	2.5
1	A	60	ALA	2.5
1	A	189	ALA	2.5
1	B	285	VAL	2.5
1	C	285	VAL	2.5
1	B	7	ILE	2.5
1	B	187	SER	2.5
1	A	183	CYS	2.5
1	B	218	ALA	2.5
1	D	218	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	44	VAL	2.5
1	B	99	SER	2.5
1	B	295	VAL	2.5
1	D	174	LYS	2.5
1	D	75	GLU	2.5
1	B	127	GLY	2.5
1	C	79	ASN	2.5
1	A	75	GLU	2.5
1	B	284	ALA	2.5
1	A	289	TRP	2.5
1	C	187	SER	2.5
1	C	102	PRO	2.5
1	A	153	VAL	2.5
1	B	111	VAL	2.5
1	B	161	ILE	2.5
1	B	198	CYS	2.4
1	D	179	LEU	2.4
1	C	54	ASN	2.4
1	A	185	MET	2.4
1	A	89	LYS	2.4
1	B	196	VAL	2.4
1	C	232	PHE	2.4
1	A	55	GLN	2.4
1	B	143	SER	2.4
1	B	167	THR	2.4
1	B	200	LEU	2.4
1	B	249	LEU	2.4
1	A	74	VAL	2.4
1	A	257	VAL	2.4
1	C	134	GLY	2.4
1	A	109	ALA	2.4
1	A	233	ALA	2.4
1	C	282	MET	2.4
1	D	227	ILE	2.4
1	C	97	MET	2.4
1	A	265	ALA	2.4
1	B	41	ALA	2.4
1	B	40	VAL	2.3
1	B	38	ALA	2.3
1	A	96	ASP	2.3
1	B	231	ASP	2.3
1	C	183	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	13	GLY	2.3
1	B	12	LEU	2.3
1	C	106	LEU	2.3
1	C	203	GLU	2.3
1	C	83	GLY	2.3
1	D	245	LEU	2.3
1	C	209	ILE	2.3
1	D	121	ASP	2.3
1	A	115	LYS	2.3
1	B	130	GLY	2.3
1	C	11	GLY	2.3
1	A	261	MET	2.3
1	D	264[A]	MET	2.3
1	D	70	ASN	2.3
1	D	79	ASN	2.3
1	B	157	ILE	2.3
1	C	196	VAL	2.3
1	A	269	PHE	2.3
1	C	103	SER	2.3
1	A	154	LEU	2.3
1	A	205	MET	2.3
1	C	259	LEU	2.3
1	A	248	ALA	2.3
1	B	28	VAL	2.3
1	B	153	VAL	2.3
1	C	74	VAL	2.3
1	C	101	SER	2.3
1	C	96	ASP	2.3
1	D	118	ASP	2.3
1	D	166	ASP	2.3
1	A	69	PRO	2.2
1	D	71	ALA	2.2
1	D	295	VAL	2.2
1	B	37	GLU	2.2
1	A	245	LEU	2.2
1	B	245	LEU	2.2
1	B	225	LYS	2.2
1	C	175	ILE	2.2
1	D	231	ASP	2.2
1	A	100	VAL	2.2
1	B	88	CYS	2.2
1	C	198	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	243	LYS	2.2
1	A	192	LEU	2.2
1	B	292	MET	2.2
1	D	168	GLY	2.2
1	C	248	ALA	2.2
1	B	16	GLY	2.2
1	C	47	GLY	2.2
1	D	214	GLY	2.2
1	C	234	GLY	2.2
1	B	102	PRO	2.2
1	A	12	LEU	2.2
1	D	67	SER	2.2
1	B	265	ALA	2.2
1	D	265	ALA	2.2
1	A	157	ILE	2.2
1	A	77	VAL	2.2
1	B	8	GLY	2.2
1	B	136	LEU	2.2
1	B	224	GLU	2.2
1	B	183	CYS	2.2
1	D	101	SER	2.2
1	B	20	ALA	2.2
1	D	164	VAL	2.1
1	B	205	MET	2.1
1	C	283	SER	2.1
1	D	248	ALA	2.1
1	A	221	ALA	2.1
1	A	263	ALA	2.1
1	C	182	GLY	2.1
1	A	48	ALA	2.1
1	A	208	ILE	2.1
1	B	21	ILE	2.1
1	D	161	ILE	2.1
1	A	283	SER	2.1
1	C	125	SER	2.1
1	A	219	MET	2.1
1	B	181	LEU	2.1
1	A	172	ALA	2.1
1	C	289	TRP	2.1
1	C	171	ASP	2.1
1	A	161	ILE	2.1
1	A	209	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	208	ILE	2.1
1	B	297	VAL	2.1
1	B	282	MET	2.0
1	A	187	SER	2.0
1	C	279	ARG	2.0
1	A	17	LYS	2.0
1	A	147	PHE	2.0
1	C	223	MET	2.0
1	D	293	THR	2.0
1	B	131	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 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.