



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:23 PM GMT

PDB ID : 1OSI  
Title : STRUCTURE OF 3-ISOPROPYLMALATE DEHYDROGENASE  
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Deposited on : 1996-10-22  
Resolution : 3.00 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

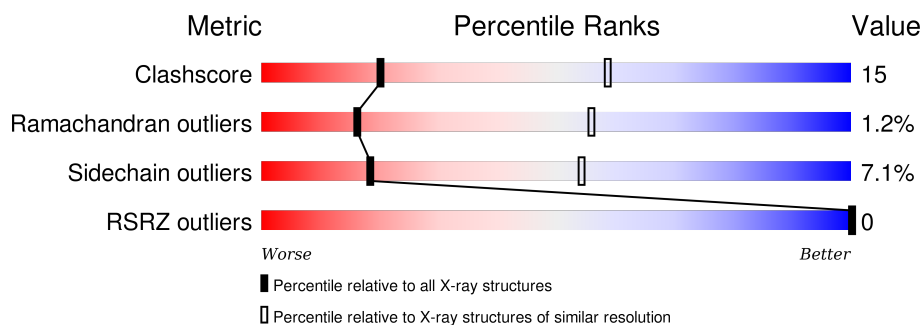
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	345	
1	B	345	
1	C	345	
1	D	345	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12572 atoms, of which 2192 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.

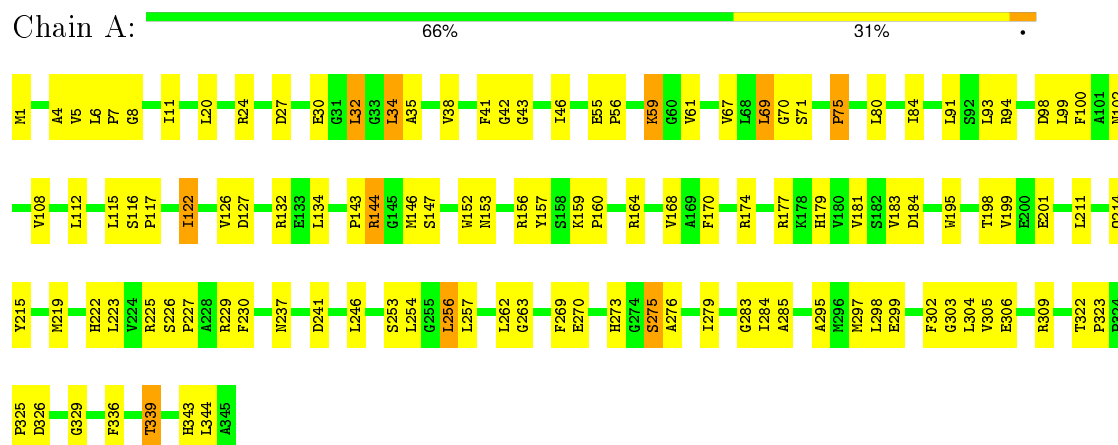
- Molecule 1 is a protein called 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	H	N	O	S	0	0	0
			3143	1654	548	452	483	6			
1	B	345	Total	C	H	N	O	S	0	0	0
			3143	1654	548	452	483	6			
1	C	345	Total	C	H	N	O	S	0	0	0
			3143	1654	548	452	483	6			
1	D	345	Total	C	H	N	O	S	0	0	0
			3143	1654	548	452	483	6			

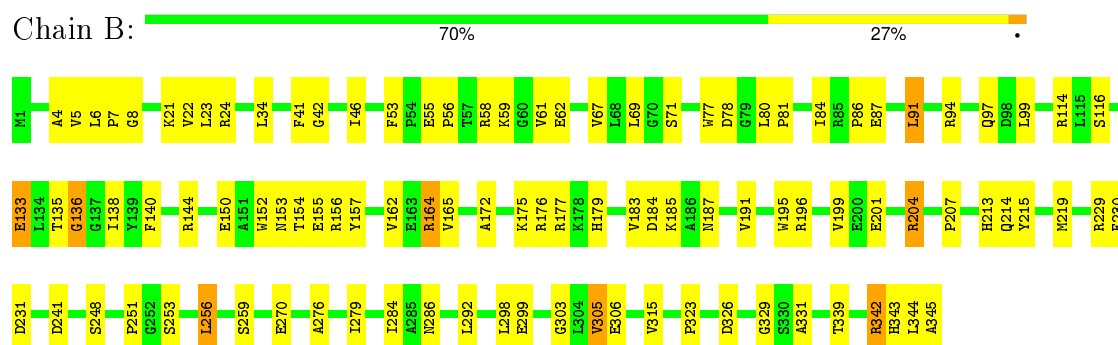
### 3 Residue-property plots

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.

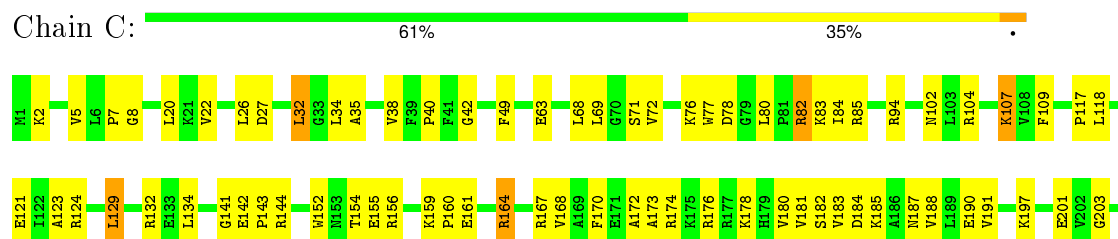
#### • Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

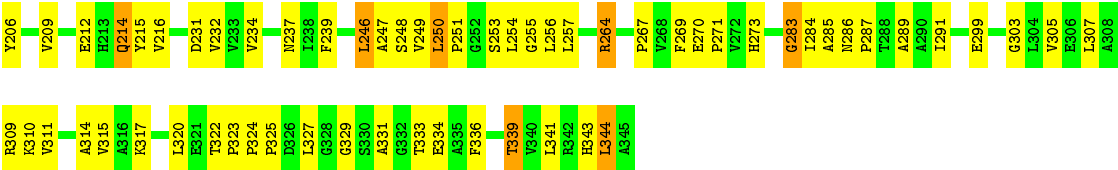


#### • Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



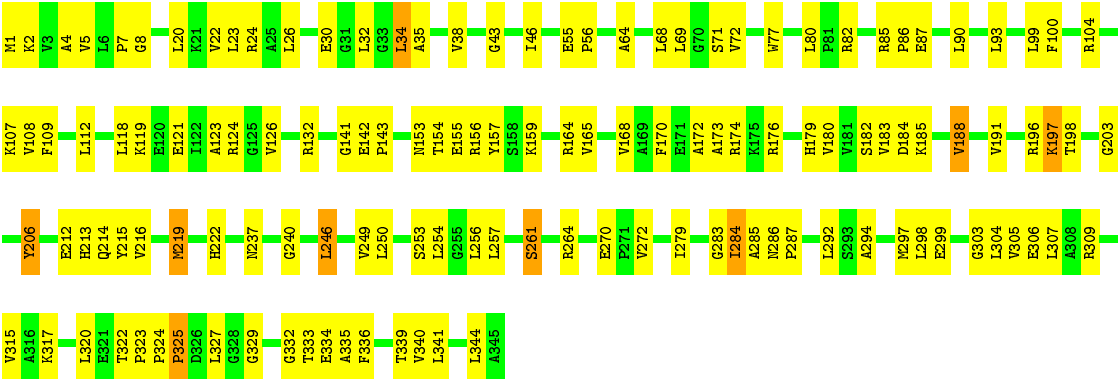
#### • Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE





● Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain D: 62% 36%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.50 Å 86.70 Å 112.10 Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00 68.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-3.00) 84.8 (68.58-3.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 3.01 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.149 , (Not available) 0.143 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 22.9	EDS
Estimated twinning fraction	0.018 for -k,-h,-l 0.028 for k,h,-l 0.397 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 27930 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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

### 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	0.38	0/2650	0.67	0/3596
1	B	0.39	0/2650	0.67	1/3596 (0.0%)
1	C	0.38	0/2650	0.64	0/3596
1	D	0.39	0/2650	0.65	0/3596
All	All	0.39	0/10600	0.66	1/14384 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	GLY	N-CA-C	6.17	128.53	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2595	548	2633	75	0
1	B	2595	548	2633	70	0
1	C	2595	548	2633	90	0
1	D	2595	548	2633	89	0
All	All	10380	2192	10532	307	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 15.

All (307) 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:153:ASN:HD22	1:C:191:VAL:HG23	1.32	0.94
1:B:204:ARG:HH11	1:B:204:ARG:HB2	1.35	0.92
1:D:287:PRO:HG3	1:D:333:THR:HG23	1.52	0.92
1:A:322:THR:OG1	1:A:339:THR:HG21	1.79	0.82
1:B:133:GLU:HG2	1:B:165:VAL:HG21	1.63	0.80
1:C:174:ARG:HA	1:C:178:LYS:HE3	1.64	0.77
1:B:80:LEU:HD23	1:B:84:ILE:HD12	1.67	0.77
1:C:78:ASP:HA	1:C:85:ARG:NH1	1.98	0.77
1:A:143:PRO:HB2	1:A:152:TRP:HE1	1.51	0.76
1:D:30:GLU:HG3	1:D:307:LEU:HD21	1.69	0.75
1:C:80:LEU:O	1:C:85:ARG:HD3	1.87	0.74
1:A:94:ARG:HD2	1:A:134:LEU:HD13	1.69	0.74
1:A:30:GLU:HB2	1:A:32:LEU:CD1	2.20	0.72
1:D:23:LEU:HB3	1:D:34:LEU:HD11	1.72	0.72
1:C:142:GLU:HG3	1:C:143:PRO:HA	1.71	0.71
1:A:5:VAL:O	1:A:7:PRO:HD3	1.90	0.71
1:D:219:MET:HE3	1:D:219:MET:HA	1.74	0.70
1:D:184:ASP:O	1:D:215:TYR:HA	1.92	0.69
1:A:91:LEU:HD22	1:A:94:ARG:HH21	1.57	0.69
1:B:153:ASN:HD22	1:D:191:VAL:HG23	1.58	0.69
1:A:4:ALA:HB3	1:A:67:VAL:HG22	1.74	0.68
1:A:100:PHE:CE1	1:A:164:ARG:HB3	2.30	0.66
1:D:43:GLY:HA2	1:D:46:ILE:HD12	1.77	0.66
1:B:201:GLU:HA	1:B:204:ARG:HD3	1.78	0.66
1:B:191:VAL:HG23	1:D:153:ASN:HD22	1.61	0.65
1:C:254:LEU:HD12	1:C:257:LEU:HD12	1.79	0.65
1:A:8:GLY:HA3	1:A:71:SER:O	1.96	0.65
1:B:116:SER:O	1:D:119:LYS:HE2	1.97	0.65
1:D:99:LEU:HD13	1:D:261:SER:HB3	1.78	0.64
1:B:299:GLU:O	1:B:303:GLY:HA2	1.98	0.63
1:D:55:GLU:HB2	1:D:56:PRO:HD3	1.81	0.63
1:C:184:ASP:O	1:C:215:TYR:HA	1.98	0.63
1:C:124:ARG:HD2	1:D:124:ARG:HD2	1.80	0.63
1:B:4:ALA:HB3	1:B:67:VAL:HG22	1.81	0.62
1:A:1:MET:HE1	1:A:32:LEU:HD23	1.80	0.62
1:B:204:ARG:HB2	1:B:204:ARG:NH1	2.12	0.62
1:C:305:VAL:O	1:C:309:ARG:HG2	1.98	0.62
1:A:253:SER:HB3	1:A:256:LEU:HD21	1.81	0.62
1:A:30:GLU:HB2	1:A:32:LEU:HD12	1.81	0.61
1:D:322:THR:HG21	1:D:339:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:O	1:A:24:ARG:HG3	1.99	0.61
1:B:8:GLY:HA3	1:B:71:SER:O	2.01	0.61
1:B:292:LEU:HD21	1:B:315:VAL:HG21	1.84	0.60
1:A:59:LYS:CD	1:A:59:LYS:N	2.65	0.59
1:C:78:ASP:HA	1:C:85:ARG:HH12	1.66	0.59
1:C:161:GLU:HA	1:C:164:ARG:HH11	1.68	0.59
1:C:118:LEU:HB2	1:C:123:ALA:HB2	1.85	0.58
1:D:196:ARG:CZ	1:D:213:HIS:HB3	2.33	0.58
1:A:323:PRO:O	1:A:329:GLY:HA3	2.03	0.58
1:A:159:LYS:HD2	1:A:198:THR:HG23	1.84	0.58
1:C:325:PRO:HD3	1:C:331:ALA:O	2.03	0.58
1:D:305:VAL:O	1:D:309:ARG:HG2	2.03	0.58
1:B:21:LYS:HD2	1:B:24:ARG:NH2	2.19	0.58
1:B:175:LYS:HD2	1:B:305:VAL:CG2	2.34	0.58
1:A:339:THR:O	1:A:343:HIS:HD2	1.86	0.57
1:D:55:GLU:H	1:D:55:GLU:CD	2.08	0.57
1:B:201:GLU:O	1:B:204:ARG:HD3	2.03	0.57
1:A:43:GLY:HA2	1:A:46:ILE:HD12	1.85	0.57
1:C:173:ALA:HB2	1:C:180:VAL:HG23	1.85	0.57
1:C:121:GLU:HA	1:C:124:ARG:HE	1.70	0.57
1:A:184:ASP:O	1:A:215:TYR:HA	2.05	0.57
1:A:1:MET:HB3	1:A:34:LEU:HA	1.87	0.56
1:D:104:ARG:HH11	1:D:272:VAL:HG21	1.70	0.56
1:B:339:THR:O	1:B:343:HIS:HD2	1.88	0.56
1:C:253:SER:OG	1:C:256:LEU:HD13	2.05	0.56
1:C:264:ARG:HH11	1:C:264:ARG:HG3	1.71	0.56
1:B:276:ALA:O	1:B:279:ILE:HG22	2.06	0.56
1:C:246:LEU:O	1:C:249:VAL:HG22	2.07	0.55
1:D:69:LEU:HD21	1:D:90:LEU:HD21	1.87	0.55
1:D:197:LYS:HZ3	1:D:198:THR:HA	1.70	0.55
1:C:82:ARG:HA	1:C:85:ARG:HG2	1.88	0.55
1:A:127:ASP:O	1:A:177:ARG:NH2	2.40	0.55
1:D:8:GLY:HA3	1:D:71:SER:O	2.07	0.55
1:C:285:ALA:O	1:C:287:PRO:HD3	2.07	0.55
1:A:153:ASN:ND2	1:C:191:VAL:HG23	2.13	0.54
1:D:206:TYR:N	1:D:206:TYR:CD1	2.75	0.54
1:D:325:PRO:HA	1:D:329:GLY:O	2.07	0.54
1:C:2:LYS:HA	1:C:35:ALA:O	2.07	0.54
1:D:5:VAL:O	1:D:7:PRO:HD3	2.07	0.54
1:C:286:ASN:ND2	1:C:324:PRO:HG3	2.23	0.54
1:A:61:VAL:HB	1:A:67:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLU:CD	1:A:306:GLU:H	2.10	0.54
1:D:304:LEU:HD23	1:D:307:LEU:HD12	1.89	0.54
1:A:27:ASP:HA	1:A:32:LEU:HD13	1.90	0.54
1:D:107:LYS:HD3	1:D:109:PHE:CE1	2.42	0.54
1:B:177:ARG:HH11	1:B:177:ARG:HG3	1.73	0.54
1:D:185:LYS:HD3	1:D:216:VAL:HG12	1.89	0.54
1:B:97:GLN:HB2	1:B:99:LEU:HG	1.90	0.54
1:C:214:GLN:HA	1:C:214:GLN:HE21	1.72	0.53
1:B:55:GLU:H	1:B:55:GLU:CD	2.12	0.53
1:B:53:PHE:CE2	1:B:58:ARG:HG2	2.43	0.53
1:B:175:LYS:HD2	1:B:305:VAL:HG22	1.90	0.53
1:D:323:PRO:O	1:D:329:GLY:HA3	2.07	0.53
1:A:299:GLU:O	1:A:303:GLY:HA2	2.09	0.53
1:D:219:MET:HA	1:D:219:MET:CE	2.38	0.53
1:C:141:GLY:HA3	1:C:154:THR:O	2.08	0.53
1:B:153:ASN:ND2	1:D:191:VAL:HG23	2.22	0.53
1:A:55:GLU:OE1	1:A:59:LYS:HE2	2.08	0.53
1:B:195:TRP:O	1:B:199:VAL:HG23	2.08	0.53
1:C:161:GLU:HA	1:C:164:ARG:NH1	2.23	0.53
1:D:72:VAL:HG22	1:D:86:PRO:HB2	1.91	0.52
1:B:140:PHE:HA	1:B:144:ARG:HH12	1.74	0.52
1:D:298:LEU:HD22	1:D:304:LEU:HD22	1.90	0.52
1:B:342:ARG:HH11	1:B:342:ARG:HG2	1.74	0.52
1:B:323:PRO:O	1:B:329:GLY:HA3	2.10	0.52
1:D:197:LYS:HG3	1:D:198:THR:N	2.23	0.52
1:C:267:PRO:HB2	1:C:269:PHE:CE1	2.44	0.52
1:C:8:GLY:HA3	1:C:71:SER:O	2.09	0.52
1:A:112:LEU:HB3	1:A:115:LEU:HD12	1.92	0.52
1:B:55:GLU:N	1:B:56:PRO:HD2	2.24	0.52
1:C:187:ASN:ND2	1:C:188:VAL:HG13	2.25	0.52
1:D:141:GLY:HA3	1:D:154:THR:O	2.10	0.52
1:D:165:VAL:O	1:D:168:VAL:HG22	2.09	0.52
1:D:246:LEU:O	1:D:249:VAL:HG22	2.10	0.52
1:C:42:GLY:HA3	1:C:72:VAL:HG23	1.91	0.51
1:D:22:VAL:HA	1:D:341:LEU:HD21	1.91	0.51
1:C:107:LYS:HD3	1:C:109:PHE:CE1	2.46	0.51
1:D:306:GLU:CD	1:D:306:GLU:H	2.14	0.51
1:D:2:LYS:HA	1:D:35:ALA:O	2.10	0.51
1:A:305:VAL:O	1:A:309:ARG:HG2	2.10	0.51
1:D:69:LEU:HB3	1:D:270:GLU:HB3	1.93	0.51
1:A:146:MET:HG2	1:A:147:SER:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ALA:O	1:C:176:ARG:HG3	2.11	0.51
1:C:322:THR:OG1	1:C:339:THR:HG21	2.10	0.51
1:D:174:ARG:HE	1:D:206:TYR:HD2	1.56	0.51
1:B:201:GLU:HA	1:B:204:ARG:CD	2.41	0.50
1:B:5:VAL:O	1:B:7:PRO:HD3	2.11	0.50
1:C:181:VAL:HG13	1:C:212:GLU:HG3	1.94	0.50
1:D:179:HIS:CE1	1:D:212:GLU:HG3	2.46	0.50
1:A:30:GLU:HB2	1:A:32:LEU:HD11	1.93	0.50
1:A:6:LEU:HD23	1:A:41:PHE:CG	2.46	0.50
1:C:311:VAL:O	1:C:315:VAL:HG23	2.10	0.50
1:D:26:LEU:HD13	1:D:344:LEU:HD21	1.93	0.50
1:C:248:SER:O	1:C:251:PRO:HD2	2.12	0.50
1:C:94:ARG:NH1	1:C:94:ARG:HB2	2.26	0.50
1:C:83:LYS:HG3	1:C:84:ILE:HG12	1.94	0.50
1:C:183:VAL:HA	1:C:214:GLN:O	2.12	0.49
1:B:80:LEU:HD23	1:B:84:ILE:CD1	2.41	0.49
1:A:256:LEU:N	1:A:256:LEU:HD23	2.28	0.49
1:D:159:LYS:HZ1	1:D:197:LYS:HZ1	1.60	0.49
1:D:179:HIS:HE1	1:D:212:GLU:HG3	1.77	0.49
1:B:187:ASN:HB3	1:B:215:TYR:CZ	2.48	0.49
1:A:42:GLY:O	1:A:46:ILE:HG13	2.12	0.49
1:A:160:PRO:O	1:A:164:ARG:HG3	2.13	0.49
1:B:172:ALA:O	1:B:176:ARG:HG3	2.13	0.49
1:C:314:ALA:CB	1:C:344:LEU:HD22	2.43	0.49
1:A:153:ASN:HD21	1:C:190:GLU:N	2.11	0.49
1:C:299:GLU:O	1:C:303:GLY:HA2	2.13	0.48
1:C:182:SER:HA	1:C:234:VAL:HG13	1.95	0.48
1:B:183:VAL:HA	1:B:214:GLN:O	2.13	0.48
1:A:11:ILE:HG12	1:A:275:SER:O	2.13	0.48
1:C:40:PRO:HG3	1:C:49:PHE:HE1	1.78	0.48
1:C:27:ASP:HA	1:C:32:LEU:HD22	1.94	0.48
1:C:82:ARG:HA	1:C:85:ARG:CG	2.44	0.48
1:D:317:LYS:HA	1:D:320:LEU:HD23	1.93	0.48
1:A:159:LYS:HB3	1:A:160:PRO:HD3	1.95	0.48
1:B:164:ARG:HH11	1:B:164:ARG:CG	2.25	0.48
1:D:109:PHE:HB2	1:D:112:LEU:HD13	1.95	0.48
1:C:76:LYS:HD2	1:C:77:TRP:NE1	2.29	0.48
1:C:310:LYS:HE2	1:C:344:LEU:O	2.14	0.48
1:B:248:SER:O	1:B:251:PRO:HD2	2.13	0.48
1:B:91:LEU:HD12	1:B:94:ARG:HH12	1.80	0.47
1:D:85:ARG:HD2	1:D:87:GLU:OE1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HD22	1:C:307:LEU:CD2	2.44	0.47
1:A:297:MET:SD	1:A:302:PHE:HE2	2.38	0.47
1:B:150:GLU:HB2	1:D:157:TYR:O	2.14	0.47
1:C:197:LYS:O	1:C:201:GLU:HG3	2.15	0.47
1:A:108:VAL:HG23	1:A:126:VAL:HB	1.96	0.47
1:C:5:VAL:O	1:C:38:VAL:HA	2.15	0.47
1:D:294:ALA:O	1:D:297:MET:HB3	2.15	0.47
1:D:172:ALA:O	1:D:176:ARG:HG3	2.15	0.47
1:B:306:GLU:CD	1:B:306:GLU:H	2.18	0.46
1:D:286:ASN:ND2	1:D:324:PRO:HG3	2.30	0.46
1:D:159:LYS:NZ	1:D:197:LYS:HZ1	2.13	0.46
1:C:77:TRP:HA	1:C:80:LEU:HD13	1.98	0.46
1:D:77:TRP:HB3	1:D:80:LEU:HD12	1.97	0.46
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.75	0.46
1:C:178:LYS:O	1:C:209:VAL:HG13	2.16	0.46
1:B:259:SER:HB3	1:B:270:GLU:O	2.15	0.46
1:C:76:LYS:O	1:C:76:LYS:HG2	2.15	0.46
1:D:143:PRO:HD2	1:D:156:ARG:HH21	1.80	0.46
1:A:183:VAL:HA	1:A:214:GLN:O	2.16	0.46
1:A:276:ALA:O	1:A:279:ILE:HG22	2.16	0.46
1:D:332:GLY:O	1:D:335:ALA:HB3	2.16	0.46
1:D:108:VAL:HG23	1:D:126:VAL:HB	1.98	0.46
1:B:184:ASP:O	1:B:215:TYR:HA	2.15	0.46
1:A:253:SER:CB	1:A:256:LEU:HD21	2.45	0.46
1:A:153:ASN:ND2	1:C:191:VAL:H	2.13	0.46
1:C:124:ARG:NH1	1:D:121:GLU:HA	2.31	0.46
1:D:254:LEU:HD12	1:D:257:LEU:HD12	1.97	0.46
1:A:59:LYS:N	1:A:59:LYS:HD2	2.31	0.45
1:B:23:LEU:HD21	1:B:298:LEU:HD21	1.98	0.45
1:B:343:HIS:C	1:B:345:ALA:H	2.18	0.45
1:C:104:ARG:HB3	1:C:104:ARG:HH11	1.81	0.45
1:D:219:MET:HE2	1:D:222:HIS:HB2	1.98	0.45
1:C:124:ARG:NH2	1:D:124:ARG:HH21	2.14	0.45
1:B:114:ARG:HG2	1:B:114:ARG:HH11	1.79	0.45
1:C:216:VAL:HG21	1:C:239:PHE:CD1	2.51	0.45
1:C:247:ALA:HA	1:C:250:LEU:HD22	1.97	0.45
1:D:5:VAL:O	1:D:38:VAL:HA	2.16	0.45
1:B:42:GLY:O	1:B:46:ILE:HG13	2.16	0.45
1:B:185:LYS:HA	1:B:185:LYS:HD2	1.73	0.45
1:B:253:SER:HB3	1:B:256:LEU:HG	1.99	0.45
1:B:6:LEU:HD23	1:B:41:PHE:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TRP:O	1:B:80:LEU:HD13	2.17	0.45
1:A:102:ASN:HB3	1:A:132:ARG:HG3	1.98	0.45
1:D:299:GLU:CD	1:D:309:ARG:HH22	2.21	0.45
1:D:299:GLU:O	1:D:303:GLY:HA2	2.17	0.45
1:D:320:LEU:O	1:D:323:PRO:HD3	2.16	0.45
1:B:80:LEU:HB3	1:B:81:PRO:CD	2.47	0.44
1:D:118:LEU:HB2	1:D:123:ALA:HB2	1.98	0.44
1:B:201:GLU:CA	1:B:204:ARG:HD3	2.47	0.44
1:C:76:LYS:HD2	1:C:77:TRP:CE2	2.53	0.44
1:A:116:SER:HA	1:A:117:PRO:HD3	1.89	0.44
1:D:183:VAL:HA	1:D:214:GLN:O	2.17	0.44
1:A:179:HIS:NE2	1:A:181:VAL:HG22	2.31	0.44
1:A:55:GLU:N	1:A:56:PRO:HD2	2.32	0.44
1:C:181:VAL:HG22	1:C:212:GLU:HG2	1.99	0.44
1:D:283:GLY:O	1:D:285:ALA:N	2.50	0.44
1:C:129:LEU:HD23	1:C:232:VAL:HG13	1.99	0.44
1:A:336:PHE:O	1:A:339:THR:HG23	2.16	0.44
1:C:264:ARG:NH1	1:C:264:ARG:HG3	2.32	0.44
1:A:222:HIS:CE1	1:A:225:ARG:HH21	2.36	0.44
1:B:154:THR:HG21	1:B:156:ARG:NH2	2.33	0.44
1:D:304:LEU:HD23	1:D:307:LEU:CD1	2.49	0.43
1:A:80:LEU:HD13	1:A:84:ILE:HD12	2.00	0.43
1:A:1:MET:CE	1:A:32:LEU:HD23	2.46	0.43
1:B:61:VAL:HG23	1:B:67:VAL:CG2	2.49	0.43
1:B:177:ARG:NH2	1:B:230:PHE:O	2.51	0.43
1:A:262:LEU:HD12	1:A:262:LEU:N	2.34	0.43
1:D:292:LEU:HD21	1:D:315:VAL:HG11	2.00	0.43
1:D:159:LYS:NZ	1:D:198:THR:HG23	2.33	0.43
1:D:104:ARG:NH1	1:D:272:VAL:HG11	2.33	0.43
1:C:283:GLY:O	1:C:285:ALA:N	2.51	0.43
1:C:5:VAL:O	1:C:7:PRO:HD3	2.19	0.43
1:D:253:SER:OG	1:D:256:LEU:HG	2.18	0.43
1:D:100:PHE:CE2	1:D:164:ARG:HD2	2.53	0.43
1:D:173:ALA:HB2	1:D:180:VAL:HG23	2.01	0.43
1:A:144:ARG:HA	1:A:152:TRP:O	2.18	0.43
1:C:124:ARG:NH2	1:D:124:ARG:NH2	2.67	0.43
1:D:322:THR:CG2	1:D:339:THR:HG21	2.48	0.43
1:D:100:PHE:CD2	1:D:164:ARG:HD2	2.54	0.42
1:A:254:LEU:HD23	1:A:257:LEU:HD12	2.01	0.42
1:B:94:ARG:HA	1:B:99:LEU:HD12	2.00	0.42
1:B:183:VAL:HG21	1:B:219:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HG23	1:B:67:VAL:HG21	1.99	0.42
1:B:86:PRO:HG2	1:B:87:GLU:OE1	2.19	0.42
1:B:153:ASN:ND2	1:D:191:VAL:H	2.17	0.42
1:D:4:ALA:HB2	1:D:64:ALA:HB2	2.00	0.42
1:D:284:ILE:HG22	1:D:325:PRO:HG2	2.02	0.42
1:A:156:ARG:HG3	1:C:152:TRP:HB3	2.01	0.42
1:C:159:LYS:N	1:C:160:PRO:CD	2.83	0.42
1:A:223:LEU:O	1:A:227:PRO:HB3	2.19	0.42
1:D:174:ARG:NE	1:D:206:TYR:HD2	2.18	0.42
1:C:5:VAL:HG11	1:C:20:LEU:HD11	2.02	0.42
1:C:174:ARG:HE	1:C:206:TYR:HD2	1.66	0.42
1:A:7:PRO:O	1:A:70:GLY:HA3	2.19	0.42
1:B:144:ARG:HA	1:B:152:TRP:O	2.20	0.42
1:B:342:ARG:NH1	1:B:342:ARG:HG2	2.34	0.42
1:C:84:ILE:O	1:C:84:ILE:HG22	2.19	0.42
1:C:102:ASN:HB2	1:C:134:LEU:HD21	2.02	0.42
1:C:339:THR:O	1:C:343:HIS:CD2	2.73	0.42
1:C:271:PRO:HB2	1:C:273:HIS:CD2	2.55	0.42
1:C:327:LEU:HA	1:C:327:LEU:HD12	1.89	0.42
1:C:287:PRO:O	1:C:291:ILE:HG13	2.20	0.42
1:C:69:LEU:HB3	1:C:270:GLU:HB3	2.01	0.42
1:A:99:LEU:HA	1:A:263:GLY:HA3	2.02	0.42
1:C:287:PRO:HD3	1:C:333:THR:HG23	2.01	0.42
1:A:122:ILE:H	1:A:122:ILE:HG12	1.67	0.42
1:B:204:ARG:O	1:B:207:PRO:HD3	2.20	0.41
1:C:22:VAL:HA	1:C:341:LEU:HD21	2.01	0.41
1:B:59:LYS:HA	1:B:62:GLU:HB2	2.02	0.41
1:D:26:LEU:HD13	1:D:344:LEU:CD2	2.50	0.41
1:A:69:LEU:HB3	1:A:270:GLU:HB3	2.02	0.41
1:D:170:PHE:CZ	1:D:203:GLY:HA2	2.54	0.41
1:D:20:LEU:O	1:D:24:ARG:HG3	2.20	0.41
1:A:152:TRP:HB3	1:C:156:ARG:HG3	2.02	0.41
1:A:283:GLY:O	1:A:285:ALA:N	2.53	0.41
1:C:255:GLY:O	1:C:289:ALA:HB2	2.21	0.41
1:C:167:ARG:HG2	1:C:206:TYR:OH	2.20	0.41
1:A:91:LEU:HD22	1:A:94:ARG:NH2	2.31	0.41
1:D:132:ARG:HD2	1:D:240:GLY:C	2.40	0.41
1:C:336:PHE:O	1:C:339:THR:HG23	2.20	0.41
1:A:219:MET:HE3	1:A:230:PHE:CZ	2.56	0.41
1:A:226:SER:O	1:A:229:ARG:HG2	2.20	0.41
1:A:122:ILE:HD11	1:C:117:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:PHE:CZ	1:C:203:GLY:HA2	2.56	0.41
1:B:138:ILE:HA	1:B:155:GLU:HA	2.02	0.41
1:B:53:PHE:CZ	1:B:58:ARG:HA	2.56	0.41
1:B:162:VAL:HG22	1:B:195:TRP:CZ3	2.56	0.41
1:D:341:LEU:HD23	1:D:341:LEU:HA	1.83	0.41
1:C:176:ARG:NH1	1:C:231:ASP:OD1	2.54	0.41
1:A:269:PHE:CE2	1:A:297:MET:HA	2.56	0.41
1:A:195:TRP:O	1:A:199:VAL:HG23	2.20	0.41
1:B:179:HIS:O	1:B:231:ASP:HB3	2.21	0.41
1:A:170:PHE:CZ	1:A:211:LEU:HD13	2.56	0.41
1:D:1:MET:CE	1:D:34:LEU:HG	2.51	0.41
1:B:196:ARG:HG3	1:B:213:HIS:CE1	2.56	0.40
1:D:104:ARG:NH1	1:D:272:VAL:HG21	2.35	0.40
1:B:177:ARG:HG3	1:B:177:ARG:NH1	2.34	0.40
1:A:59:LYS:HD2	1:A:59:LYS:HA	1.92	0.40
1:C:102:ASN:HB3	1:C:132:ARG:HG3	2.03	0.40
1:A:295:ALA:HA	1:A:298:LEU:HD12	2.04	0.40
1:C:256:LEU:HD12	1:C:256:LEU:N	2.37	0.40
1:C:323:PRO:O	1:C:329:GLY:HA3	2.20	0.40
1:B:22:VAL:HG13	1:B:344:LEU:HD21	2.04	0.40
1:D:336:PHE:O	1:D:340:VAL:HG23	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	343/345 (99%)	312 (91%)	27 (8%)	4 (1%)	16	56
1	B	343/345 (99%)	309 (90%)	29 (8%)	5 (2%)	13	50
1	C	343/345 (99%)	317 (92%)	22 (6%)	4 (1%)	16	56
1	D	343/345 (99%)	314 (92%)	25 (7%)	4 (1%)	16	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1372/1380 (99%)	1252 (91%)	103 (8%)	17 (1%)	16	56

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	THR
1	B	136	GLY
1	C	82	ARG
1	C	284	ILE
1	D	82	ARG
1	D	284	ILE
1	A	35	ALA
1	A	284	ILE
1	B	284	ILE
1	B	305	VAL
1	A	237	ASN
1	C	237	ASN
1	B	331	ALA
1	D	237	ASN
1	C	283	GLY
1	A	75	PRO
1	D	188	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/266 (100%)	243 (91%)	23 (9%)	13	44
1	B	266/266 (100%)	252 (95%)	14 (5%)	28	67
1	C	266/266 (100%)	246 (92%)	20 (8%)	17	51
1	D	266/266 (100%)	247 (93%)	19 (7%)	18	54
All	All	1064/1064 (100%)	988 (93%)	76 (7%)	18	54

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



Mol	Chain	Res	Type
1	A	32	LEU
1	A	34	LEU
1	A	38	VAL
1	A	59	LYS
1	A	69	LEU
1	A	75	PRO
1	A	93	LEU
1	A	98	ASP
1	A	122	ILE
1	A	144	ARG
1	A	157	TYR
1	A	168	VAL
1	A	174	ARG
1	A	201	GLU
1	A	241	ASP
1	A	246	LEU
1	A	256	LEU
1	A	273	HIS
1	A	275	SER
1	A	304	LEU
1	A	325	PRO
1	A	326	ASP
1	A	339	THR
1	B	34	LEU
1	B	69	LEU
1	B	78	ASP
1	B	91	LEU
1	B	133	GLU
1	B	157	TYR
1	B	164	ARG
1	B	204	ARG
1	B	229	ARG
1	B	241	ASP
1	B	256	LEU
1	B	286	ASN
1	B	326	ASP
1	B	342	ARG
1	C	32	LEU
1	C	34	LEU
1	C	63	GLU
1	C	68	LEU
1	C	107	LYS
1	C	129	LEU

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Mol	Chain	Res	Type
1	C	144	ARG
1	C	155	GLU
1	C	164	ARG
1	C	168	VAL
1	C	185	LYS
1	C	214	GLN
1	C	246	LEU
1	C	250	LEU
1	C	264	ARG
1	C	317	LYS
1	C	320	LEU
1	C	334	GLU
1	C	339	THR
1	C	344	LEU
1	D	32	LEU
1	D	34	LEU
1	D	68	LEU
1	D	93	LEU
1	D	142	GLU
1	D	155	GLU
1	D	182	SER
1	D	188	VAL
1	D	197	LYS
1	D	206	TYR
1	D	219	MET
1	D	246	LEU
1	D	250	LEU
1	D	261	SER
1	D	264	ARG
1	D	279	ILE
1	D	325	PRO
1	D	327	LEU
1	D	334	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	213	HIS
1	A	343	HIS
1	B	102	ASN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	286	ASN
1	B	343	HIS
1	C	153	ASN
1	C	343	HIS
1	D	153	ASN

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	345/345 (100%)	-0.88	0 100 100	8, 23, 43, 60	0
1	B	345/345 (100%)	-0.88	0 100 100	7, 23, 41, 58	0
1	C	345/345 (100%)	-0.87	0 100 100	7, 26, 45, 56	0
1	D	345/345 (100%)	-0.85	0 100 100	7, 25, 48, 62	0
All	All	1380/1380 (100%)	-0.87	0 100 100	7, 24, 44, 62	0

There are no RSRZ outliers to report.

### 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.