



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:59 PM GMT

PDB ID : 3VPX  
Title : Crystal structure of leucine dehydrogenase from a psychrophilic bacterium *Sporosarcina psychrophila*.  
Authors : Zhao, Y.; Wakamatsu, T.; Doi, K.; Sakuraba, H.; Ohshima, T.  
Deposited on : 2012-03-14  
Resolution : 2.55 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

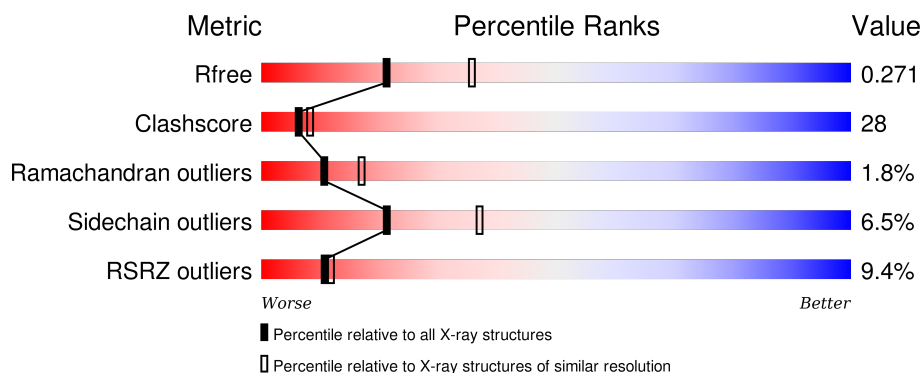
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	364	<div> <div>10%</div> <div>54%</div> <div>39%</div> <div>5%</div> </div>
1	B	364	<div> <div>9%</div> <div>55%</div> <div>39%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5517 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.

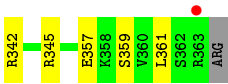
- Molecule 1 is a protein called Leucine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2718	1702	464	540	12			
1	B	359	Total	C	N	O	S	0	0	0
			2732	1710	467	543	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	30	Total	O	0	0
			30	30		





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.59Å 135.59Å 123.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.78 – 2.55 31.78 – 2.55	Depositor EDS
% Data completeness (in resolution range)	87.7 (31.78-2.55) 96.4 (31.78-2.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.63 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.290 0.259 , 0.271	Depositor DCC
$R_{free}$ test set	1752 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.6	EDS
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 35229 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5517	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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	0.39	1/2757 (0.0%)	0.63	0/3729
1	B	0.38	0/2771	0.64	0/3748
All	All	0.39	1/5528 (0.0%)	0.63	0/7477

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	C-N	-5.85	1.20	1.34

There are no bond angle outliers.

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	2718	0	2680	147	0
1	B	2732	0	2693	157	0
2	A	37	0	0	1	0
2	B	30	0	0	1	0
All	All	5517	0	5373	301	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 28.

All (301) 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:B:66:THR:HG22	1:B:78:GLY:HA3	1.41	1.03
1:A:32:HIS:ND1	1:A:66:THR:HG21	1.73	1.02
1:B:319:LYS:HD2	1:B:338:MET:HE2	1.36	1.01
1:B:154:ILE:HD11	1:B:188:LEU:HD13	1.44	0.98
1:B:204:ILE:HD12	1:B:204:ILE:H	1.34	0.92
1:A:201:ILE:HD11	1:A:213:VAL:HG23	1.51	0.92
1:B:32:HIS:ND1	1:B:66:THR:HG21	1.88	0.89
1:A:233:ILE:HG13	1:A:255:VAL:HB	1.56	0.88
1:B:151:ALA:O	1:B:154:ILE:HD13	1.75	0.85
1:A:272:LEU:HA	1:A:275:GLU:HG2	1.58	0.85
1:A:244:ASN:O	1:A:248:ILE:HG12	1.76	0.84
1:A:165:ALA:HB2	1:A:279:VAL:HG21	1.60	0.84
1:B:242:ILE:HD12	1:B:243:ILE:HG12	1.60	0.83
1:B:205:ASN:ND2	1:B:208:ALA:H	1.77	0.83
1:B:158:MET:CE	1:B:192:LEU:HD21	2.11	0.80
1:B:205:ASN:HD22	1:B:208:ALA:H	1.27	0.80
1:A:248:ILE:HB	1:A:249:PRO:HD3	1.62	0.80
1:A:234:PHE:CE2	1:A:236:PRO:HG3	2.17	0.80
1:A:363:ARG:HD2	1:A:363:ARG:H	1.46	0.77
1:A:302:ASN:HD22	1:A:305:ARG:HB2	1.49	0.76
1:A:329:ILE:HD12	1:A:333:VAL:HG12	1.66	0.76
1:A:255:VAL:HG22	1:A:279:VAL:HB	1.69	0.75
1:B:177:ALA:HA	1:B:200:ILE:HG23	1.68	0.74
1:A:289:GLY:HA2	1:A:310:VAL:HG22	1.70	0.74
1:A:302:ASN:ND2	1:A:305:ARG:H	1.85	0.74
1:B:43:THR:HG21	1:B:99:PHE:HE2	1.52	0.73
1:B:213:VAL:HA	1:B:218:ALA:HB3	1.71	0.73
1:A:125:LEU:O	1:A:128:LEU:HB2	1.88	0.72
1:B:247:THR:O	1:B:251:LEU:HG	1.89	0.71
1:A:265:LYS:HB3	1:A:269:HIS:CE1	2.24	0.71
1:A:302:ASN:HD22	1:A:305:ARG:CB	2.03	0.71
1:A:50:SER:OG	1:A:53:GLU:HB2	1.90	0.70
1:B:307:LEU:O	1:B:310:VAL:HG12	1.91	0.69
1:B:66:THR:CG2	1:B:78:GLY:HA3	2.19	0.69
1:B:255:VAL:HG22	1:B:279:VAL:CG2	2.22	0.69
1:A:147:SER:HB2	1:A:148:PRO:HD3	1.73	0.69
1:A:43:THR:HG22	1:A:112:THR:OG1	1.93	0.69
1:B:309:ARG:O	1:B:309:ARG:HD3	1.93	0.69
1:B:158:MET:HE3	1:B:192:LEU:HD21	1.75	0.69
1:B:114:GLU:HA	1:B:118:THR:CG2	2.22	0.69
1:B:205:ASN:O	1:B:209:VAL:HG23	1.93	0.68
1:B:228:SER:O	1:B:229:GLN:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:O	1:A:203:ASP:HB2	1.92	0.68
1:A:202:THR:HG21	1:A:223:ILE:HA	1.74	0.68
1:A:176:VAL:HG13	1:A:233:ILE:HG22	1.73	0.68
1:A:336:ASP:O	1:A:340:GLU:HG3	1.94	0.67
1:A:161:ALA:HB1	1:A:255:VAL:HG11	1.75	0.67
1:A:201:ILE:HD11	1:A:213:VAL:CG2	2.25	0.67
1:A:228:SER:OG	1:A:250:GLN:HB3	1.95	0.66
1:B:205:ASN:HD22	1:B:208:ALA:N	1.91	0.66
1:A:44:ARG:HD2	1:A:116:VAL:HG22	1.77	0.66
1:B:205:ASN:HD22	1:B:208:ALA:CB	2.08	0.66
1:B:200:ILE:HD13	1:B:200:ILE:C	2.17	0.65
1:B:165:ALA:HB2	1:B:279:VAL:HG21	1.78	0.65
1:B:162:ALA:C	1:B:164:GLU:H	1.97	0.65
1:A:52:GLU:HG2	1:A:55:ILE:HD12	1.79	0.65
1:A:207:GLU:O	1:A:210:GLN:HB3	1.97	0.65
1:B:38:PRO:HB3	1:B:108:GLY:O	1.96	0.65
1:B:230:GLU:OE2	1:B:230:GLU:HA	1.97	0.64
1:A:163:LYS:HA	1:A:168:ASP:N	2.12	0.64
1:B:202:THR:O	1:B:203:ASP:HB2	1.95	0.64
1:A:319:LYS:O	1:A:323:ILE:HG12	1.98	0.64
1:A:313:ILE:HA	1:A:316:VAL:CG1	2.27	0.64
1:B:81:THR:HG21	1:B:99:PHE:CZ	2.32	0.64
1:B:43:THR:HG21	1:B:99:PHE:CE2	2.31	0.63
1:A:168:ASP:OD2	1:A:170:SER:HB3	1.99	0.63
1:B:155:TYR:O	1:B:159:LYS:HG3	1.97	0.63
1:A:1:MET:N	1:A:52:GLU:OE2	2.31	0.63
1:B:323:ILE:HD12	1:B:338:MET:HB2	1.79	0.63
1:A:44:ARG:HD2	1:A:116:VAL:CG2	2.29	0.63
1:A:202:THR:HG22	1:A:203:ASP:N	2.14	0.63
1:A:302:ASN:ND2	1:A:305:ARG:HB2	2.14	0.62
1:B:162:ALA:O	1:B:164:GLU:N	2.33	0.62
1:B:114:GLU:HA	1:B:118:THR:HG21	1.80	0.62
1:B:162:ALA:C	1:B:164:GLU:N	2.53	0.61
1:B:221:VAL:HG12	1:B:222:GLY:N	2.15	0.61
1:B:204:ILE:H	1:B:204:ILE:CD1	2.08	0.61
1:B:1:MET:HG2	1:B:52:GLU:OE1	2.00	0.61
1:B:205:ASN:HD22	1:B:208:ALA:HB2	1.64	0.61
1:A:81:THR:HG21	1:A:99:PHE:CZ	2.37	0.60
1:A:233:ILE:CG1	1:A:255:VAL:HB	2.28	0.60
1:B:158:MET:HE1	1:B:192:LEU:HD21	1.84	0.60
1:A:202:THR:HG22	1:A:203:ASP:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ALA:HB1	1:B:255:VAL:HG11	1.84	0.59
1:B:357:GLU:HB2	2:B:409:HOH:O	2.01	0.59
1:B:63:ARG:HA	1:B:66:THR:HG23	1.83	0.59
1:B:255:VAL:HG13	1:B:279:VAL:HG23	1.85	0.59
1:B:166:PHE:CZ	1:B:232:ASP:HB2	2.38	0.59
1:A:162:ALA:HB2	1:A:171:LEU:HD21	1.85	0.59
1:A:199:LEU:HD12	1:A:199:LEU:N	2.18	0.59
1:B:228:SER:HB3	1:B:250:GLN:HE21	1.68	0.59
1:A:181:VAL:O	1:A:181:VAL:HG12	2.03	0.58
1:A:43:THR:HB	1:A:81:THR:HB	1.84	0.58
1:A:57:ASP:OD1	1:A:60:ARG:NH1	2.36	0.58
1:B:204:ILE:N	1:B:204:ILE:HD12	2.14	0.58
1:A:269:HIS:O	1:A:273:ILE:HG23	2.02	0.58
1:B:154:ILE:HD11	1:B:188:LEU:CD1	2.28	0.58
1:B:205:ASN:ND2	1:B:208:ALA:N	2.49	0.57
1:A:145:ASN:N	1:A:145:ASN:HD22	2.02	0.57
1:B:154:ILE:CD1	1:B:188:LEU:HD13	2.27	0.57
1:B:149:VAL:HG11	1:B:293:ASN:ND2	2.19	0.57
1:A:28:ILE:HB	1:A:82:VAL:HG22	1.86	0.56
1:B:275:GLU:HA	1:B:275:GLU:OE1	2.04	0.56
1:B:312:GLY:O	1:B:316:VAL:HG23	2.06	0.55
1:B:280:TYR:O	1:B:282:PRO:HD3	2.06	0.55
1:B:10:GLN:OE1	1:B:63:ARG:HD3	2.07	0.55
1:A:213:VAL:HG13	1:A:218:ALA:O	2.07	0.55
1:A:10:GLN:HE21	1:A:12:TYR:HE1	1.53	0.55
1:B:242:ILE:CD1	1:B:243:ILE:HG12	2.32	0.55
1:B:44:ARG:HG3	1:B:116:VAL:HB	1.89	0.54
1:A:155:TYR:CZ	1:A:159:LYS:HE2	2.42	0.54
1:A:205:ASN:HD22	1:A:208:ALA:HB2	1.72	0.54
1:B:225:GLU:O	1:B:229:GLN:HG2	2.08	0.54
1:B:248:ILE:N	1:B:249:PRO:CD	2.72	0.53
1:A:265:LYS:HB3	1:A:269:HIS:HE1	1.71	0.53
1:B:145:ASN:ND2	1:B:145:ASN:O	2.41	0.53
1:A:13:GLU:OE2	1:A:33:ASP:HA	2.08	0.53
1:B:43:THR:HA	1:B:81:THR:O	2.08	0.53
1:A:162:ALA:HB2	1:A:171:LEU:CD2	2.38	0.53
1:B:57:ASP:OD1	1:B:60:ARG:NH1	2.41	0.53
1:B:255:VAL:HG12	1:B:256:ILE:N	2.24	0.53
1:A:38:PRO:HB3	1:A:108:GLY:O	2.08	0.53
1:A:272:LEU:HA	1:A:275:GLU:CG	2.33	0.53
1:B:190:GLU:HG2	1:B:216:PHE:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:CD1	1:A:212:ALA:HB3	2.39	0.53
1:A:204:ILE:HA	1:A:223:ILE:HD11	1.91	0.53
1:B:162:ALA:HB1	1:B:168:ASP:O	2.09	0.52
1:A:165:ALA:HB2	1:A:279:VAL:CG2	2.37	0.52
1:B:244:ASN:O	1:B:248:ILE:HG13	2.10	0.52
1:A:221:VAL:HG12	1:A:225:GLU:HB2	1.91	0.52
1:A:329:ILE:HD12	1:A:333:VAL:CG1	2.38	0.52
1:B:329:ILE:HD12	1:B:333:VAL:HG12	1.91	0.52
1:A:316:VAL:O	1:A:320:ILE:HG13	2.10	0.51
1:B:210:GLN:O	1:B:213:VAL:HG22	2.10	0.51
1:B:161:ALA:O	1:B:164:GLU:HB3	2.10	0.51
1:A:155:TYR:CE1	1:A:159:LYS:HE2	2.46	0.51
1:A:291:VAL:O	1:A:294:VAL:HG22	2.11	0.51
1:A:313:ILE:HA	1:A:316:VAL:HG12	1.91	0.51
1:B:176:VAL:HG22	1:B:233:ILE:HB	1.93	0.51
1:A:287:ASN:C	1:A:287:ASN:HD22	2.14	0.51
1:B:119:THR:O	1:B:122:ASP:HB2	2.11	0.51
1:B:125:LEU:O	1:B:128:LEU:HB2	2.11	0.51
1:B:154:ILE:HD13	1:B:155:TYR:H	1.76	0.51
1:B:84:ILE:O	1:B:84:ILE:HG13	2.11	0.51
1:B:165:ALA:HB1	1:B:254:LYS:HD2	1.94	0.50
1:B:182:GLY:N	1:B:185:ALA:HB3	2.26	0.50
1:A:244:ASN:HA	1:A:269:HIS:CE1	2.45	0.50
1:B:114:GLU:HA	1:B:118:THR:HG22	1.92	0.50
1:A:234:PHE:O	1:A:236:PRO:HD3	2.12	0.50
1:A:43:THR:HA	1:A:81:THR:O	2.11	0.50
1:A:232:ASP:O	1:A:233:ILE:HD12	2.12	0.49
1:A:247:THR:O	1:A:251:LEU:HG	2.13	0.49
1:B:201:ILE:HD11	1:B:209:VAL:HG13	1.95	0.49
1:A:272:LEU:N	1:A:272:LEU:HD22	2.28	0.49
1:A:16:VAL:HG13	1:B:16:VAL:HG22	1.95	0.49
1:B:342:ARG:HA	1:B:345:ARG:NH1	2.27	0.49
1:A:233:ILE:CD1	1:A:255:VAL:HB	2.43	0.49
1:B:200:ILE:HG12	1:B:219:THR:O	2.13	0.49
1:A:293:ASN:HD22	1:A:306:ALA:HB1	1.78	0.49
1:B:193:HIS:CE1	1:B:216:PHE:HA	2.47	0.49
1:B:221:VAL:CG1	1:B:222:GLY:N	2.76	0.49
1:A:63:ARG:O	1:A:66:THR:HG23	2.13	0.48
1:A:284:TYR:HA	1:A:287:ASN:HD21	1.78	0.48
1:B:195:GLU:O	1:B:195:GLU:HG2	2.12	0.48
1:A:44:ARG:CD	1:A:115:ASP:OD2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:VAL:CG1	1:B:225:GLU:HB2	2.44	0.48
1:B:181:VAL:HG23	1:B:203:ASP:HB2	1.95	0.48
1:A:44:ARG:HG3	1:A:116:VAL:HG23	1.96	0.48
1:A:316:VAL:HG23	1:A:338:MET:CE	2.44	0.48
1:B:41:GLY:HA3	1:B:79:GLY:O	2.13	0.48
1:A:221:VAL:HG12	1:A:222:GLY:N	2.29	0.48
1:A:173:GLY:N	1:A:196:GLY:O	2.42	0.47
1:B:163:LYS:HA	1:B:168:ASP:N	2.30	0.47
1:B:145:ASN:N	1:B:145:ASN:HD22	2.13	0.47
1:B:158:MET:HE3	1:B:171:LEU:HD13	1.97	0.47
1:B:227:TYR:O	1:B:251:LEU:HD23	2.15	0.47
1:A:149:VAL:HG11	1:A:293:ASN:ND2	2.30	0.47
1:A:2:GLU:HG2	1:A:5:LYS:HB2	1.97	0.47
1:B:248:ILE:HB	1:B:249:PRO:HD3	1.97	0.47
1:A:44:ARG:HD2	1:A:115:ASP:OD2	2.14	0.47
1:B:209:VAL:O	1:B:213:VAL:HG13	2.15	0.46
1:A:40:LEU:HD23	1:A:41:GLY:N	2.29	0.46
1:B:151:ALA:O	1:B:154:ILE:CD1	2.56	0.46
1:B:158:MET:HE3	1:B:192:LEU:CD2	2.43	0.46
1:A:323:ILE:HB	1:A:334:ALA:HB1	1.97	0.46
1:A:120:GLU:OE1	1:A:137:SER:O	2.33	0.46
1:B:200:ILE:HD13	1:B:201:ILE:N	2.30	0.46
1:B:201:ILE:CD1	1:B:209:VAL:HG13	2.45	0.46
1:A:204:ILE:N	1:A:204:ILE:HD12	2.31	0.46
1:A:323:ILE:O	1:A:326:ARG:HB3	2.15	0.46
1:B:213:VAL:HG23	1:B:214:ASP:N	2.31	0.46
1:B:165:ALA:HB2	1:B:279:VAL:CG2	2.45	0.46
1:B:163:LYS:HA	1:B:167:GLY:C	2.36	0.46
1:A:242:ILE:N	1:A:242:ILE:HD13	2.31	0.46
1:B:221:VAL:HG12	1:B:225:GLU:HB2	1.97	0.46
1:A:151:ALA:CB	1:A:187:ALA:HB3	2.45	0.46
1:A:156:TYR:CD2	1:A:311:GLU:HG3	2.50	0.46
1:A:179:GLN:NE2	1:A:234:PHE:HZ	2.13	0.46
1:A:204:ILE:HD13	2:A:436:HOH:O	2.15	0.46
1:A:161:ALA:CB	1:A:255:VAL:HG11	2.45	0.46
1:A:195:GLU:O	1:A:195:GLU:HG2	2.16	0.46
1:A:209:VAL:O	1:A:213:VAL:HG23	2.15	0.46
1:A:363:ARG:H	1:A:363:ARG:CD	2.15	0.46
1:B:86:ASN:HD22	1:B:86:ASN:C	2.19	0.46
1:A:13:GLU:OE2	1:A:34:THR:N	2.46	0.45
1:B:190:GLU:HG2	1:B:216:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HA	1:A:168:ASP:H	1.82	0.45
1:A:177:ALA:HB1	1:A:226:ILE:CD1	2.47	0.45
1:A:308:LYS:O	1:A:311:GLU:HB3	2.17	0.45
1:B:61:LEU:HB3	1:B:80:LYS:HG2	1.98	0.45
1:A:285:VAL:O	1:A:288:SER:HB2	2.17	0.45
1:B:93:ASP:HA	1:B:125:LEU:HD13	1.98	0.45
1:B:154:ILE:HD13	1:B:155:TYR:N	2.31	0.45
1:A:90:ASP:N	1:A:90:ASP:OD2	2.49	0.45
1:B:202:THR:O	1:B:203:ASP:CB	2.65	0.45
1:A:153:GLY:HA2	1:A:310:VAL:HG13	1.98	0.44
1:B:63:ARG:HA	1:B:66:THR:CG2	2.47	0.44
1:B:86:ASN:HD22	1:B:87:PRO:N	2.16	0.44
1:A:200:ILE:HD13	1:A:229:GLN:HB3	2.00	0.44
1:B:297:GLU:HG3	1:B:301:TYR:HB2	1.98	0.44
1:B:158:MET:O	1:B:161:ALA:HB3	2.17	0.44
1:A:181:VAL:HG23	1:A:202:THR:O	2.17	0.44
1:B:173:GLY:N	1:B:196:GLY:O	2.50	0.44
1:B:319:LYS:HB3	1:B:338:MET:CE	2.48	0.44
1:A:114:GLU:OE2	1:A:135:GLY:O	2.36	0.44
1:A:243:ILE:HB	1:A:263:GLN:O	2.17	0.44
1:A:15:LEU:HD13	1:A:59:LEU:HD21	1.98	0.44
1:A:46:TRP:CE3	1:A:47:THR:O	2.70	0.44
1:A:28:ILE:HB	1:A:82:VAL:CG2	2.48	0.44
1:A:172:ALA:HA	1:A:196:GLY:O	2.18	0.44
1:A:114:GLU:HG3	1:A:123:MET:CG	2.48	0.44
1:A:94:GLU:H	1:A:94:GLU:CD	2.21	0.44
1:B:293:ASN:HD22	1:B:306:ALA:HB1	1.83	0.44
1:B:86:ASN:HD22	1:B:87:PRO:CD	2.31	0.44
1:A:145:ASN:N	1:A:145:ASN:ND2	2.65	0.44
1:B:288:SER:C	1:B:290:GLY:N	2.71	0.44
1:B:319:LYS:HB3	1:B:338:MET:HE1	2.00	0.43
1:B:161:ALA:HB1	1:B:255:VAL:CG1	2.48	0.43
1:B:43:THR:CG2	1:B:112:THR:OG1	2.66	0.43
1:B:305:ARG:O	1:B:309:ARG:HB2	2.17	0.43
1:A:288:SER:O	1:A:290:GLY:N	2.51	0.43
1:B:207:GLU:HA	1:B:207:GLU:OE2	2.18	0.43
1:B:105:GLY:C	1:B:107:ASN:H	2.21	0.43
1:B:200:ILE:C	1:B:200:ILE:CD1	2.86	0.43
1:B:279:VAL:HG23	1:B:279:VAL:O	2.18	0.43
1:A:205:ASN:HD22	1:A:208:ALA:CB	2.31	0.43
1:B:205:ASN:ND2	1:B:208:ALA:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.91	0.43
1:B:323:ILE:CD1	1:B:338:MET:HB2	2.46	0.43
1:B:254:LYS:O	1:B:279:VAL:HG22	2.19	0.43
1:B:194:GLU:C	1:B:196:GLY:H	2.21	0.43
1:A:236:PRO:HB3	1:A:242:ILE:HG13	2.01	0.43
1:A:21:LYS:HB2	1:B:11:ASP:OD1	2.19	0.43
1:A:201:ILE:HD12	1:A:212:ALA:HB3	2.00	0.43
1:B:158:MET:CE	1:B:171:LEU:HD13	2.47	0.43
1:B:114:GLU:OE2	1:B:120:GLU:HA	2.19	0.43
1:B:288:SER:C	1:B:290:GLY:H	2.22	0.43
1:B:205:ASN:HB3	1:B:208:ALA:HB3	2.00	0.43
1:B:146:PRO:O	1:B:149:VAL:N	2.49	0.43
1:B:232:ASP:O	1:B:233:ILE:HG13	2.19	0.43
1:A:156:TYR:CE2	1:A:311:GLU:HG3	2.54	0.43
1:B:33:ASP:O	1:B:77:GLY:HA3	2.19	0.43
1:B:50:SER:O	1:B:53:GLU:HB3	2.19	0.42
1:A:271:ASP:HB2	1:A:272:LEU:HD22	2.01	0.42
1:A:159:LYS:HG3	1:A:169:ASP:O	2.19	0.42
1:B:314:TYR:C	1:B:314:TYR:CD1	2.93	0.42
1:A:341:GLU:O	1:A:345:ARG:HG3	2.19	0.42
1:A:4:PHE:HB2	1:B:51:GLU:OE2	2.19	0.42
1:B:240:GLY:C	1:B:242:ILE:H	2.22	0.42
1:B:163:LYS:HG3	1:B:163:LYS:O	2.20	0.42
1:A:200:ILE:HG21	1:A:229:GLN:HG3	2.01	0.42
1:A:363:ARG:HD2	1:A:363:ARG:N	2.26	0.42
1:B:180:GLY:HA2	1:B:203:ASP:OD2	2.20	0.42
1:B:18:CYS:HB3	1:B:102:TYR:CD2	2.54	0.42
1:B:149:VAL:HA	1:B:307:LEU:CD2	2.49	0.42
1:B:170:SER:C	1:B:172:ALA:H	2.22	0.42
1:B:92:ASN:O	1:B:95:MET:HG2	2.20	0.41
1:A:81:THR:HG21	1:A:99:PHE:CE1	2.54	0.41
1:A:145:ASN:O	1:A:145:ASN:ND2	2.53	0.41
1:A:161:ALA:HB1	1:A:255:VAL:CG1	2.48	0.41
1:A:317:ILE:O	1:A:320:ILE:HB	2.20	0.41
1:A:190:GLU:HG2	1:A:216:PHE:CZ	2.56	0.41
1:B:66:THR:CB	1:B:78:GLY:HA3	2.50	0.41
1:B:359:SER:C	1:B:361:LEU:H	2.23	0.41
1:B:228:SER:HB3	1:B:250:GLN:NE2	2.32	0.41
1:A:63:ARG:HA	1:A:66:THR:CG2	2.50	0.41
1:A:145:ASN:HA	1:A:146:PRO:HD3	1.71	0.41
1:A:61:LEU:HB2	1:A:80:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLU:OE2	1:B:135:GLY:O	2.38	0.41
1:A:44:ARG:HD3	1:A:115:ASP:OD2	2.22	0.40
1:B:255:VAL:HG22	1:B:279:VAL:HG21	2.02	0.40
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.85	0.40
1:A:153:GLY:HA2	1:A:310:VAL:CG1	2.52	0.40
1:B:94:GLU:H	1:B:94:GLU:CD	2.25	0.40
1:A:186:TYR:O	1:A:189:CYS:HB2	2.21	0.40
1:B:289:GLY:HA2	1:B:292:ILE:HD12	2.03	0.40
1:A:210:GLN:HG2	1:A:211:ARG:N	2.36	0.40
1:A:210:GLN:O	1:A:211:ARG:C	2.60	0.40
1:A:296:ASP:CG	1:A:305:ARG:HH21	2.25	0.40
1:B:166:PHE:HZ	1:B:232:ASP:HB2	1.82	0.40
1:B:313:ILE:CG2	1:B:317:ILE:HD13	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	352/364 (97%)	309 (88%)	36 (10%)	7 (2%)	9	14
1	B	355/364 (98%)	305 (86%)	44 (12%)	6 (2%)	11	18
All	All	707/728 (97%)	614 (87%)	80 (11%)	13 (2%)	11	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASP
1	A	229	GLN
1	B	174	LYS
1	B	203	ASP
1	A	90	ASP

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Mol	Chain	Res	Type
1	A	326	ARG
1	B	163	LYS
1	B	202	THR
1	A	289	GLY
1	B	328	ASN
1	A	52	GLU
1	B	300	GLY
1	A	249	PRO

### 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	278/281 (99%)	261 (94%)	17 (6%)	23	40
1	B	278/281 (99%)	259 (93%)	19 (7%)	20	34
All	All	556/562 (99%)	520 (94%)	36 (6%)	21	37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	43	THR
1	A	44	ARG
1	A	66	THR
1	A	107	ASN
1	A	128	LEU
1	A	145	ASN
1	A	150	THR
1	A	159	LYS
1	A	164	GLU
1	A	226	ILE
1	A	242	ILE
1	A	287	ASN
1	A	288	SER
1	A	310	VAL

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Mol	Chain	Res	Type
1	A	359	SER
1	A	363	ARG
1	B	19	GLN
1	B	43	THR
1	B	44	ARG
1	B	66	THR
1	B	84	ILE
1	B	86	ASN
1	B	118	THR
1	B	145	ASN
1	B	150	THR
1	B	154	ILE
1	B	169	ASP
1	B	194	GLU
1	B	200	ILE
1	B	245	ASP
1	B	250	GLN
1	B	272	LEU
1	B	302	ASN
1	B	309	ARG
1	B	327	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	75	ASN
1	A	86	ASN
1	A	107	ASN
1	A	205	ASN
1	A	287	ASN
1	A	293	ASN
1	A	302	ASN
1	B	75	ASN
1	B	86	ASN
1	B	107	ASN
1	B	145	ASN
1	B	179	GLN
1	B	205	ASN
1	B	250	GLN
1	B	293	ASN
1	B	302	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 ⓘ

### 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	356/364 (97%)	0.55	36 (10%) 9 10	23, 52, 87, 98	0
1	B	359/364 (98%)	0.63	31 (8%) 13 14	23, 51, 82, 94	0
All	All	715/728 (98%)	0.59	67 (9%) 11 12	23, 51, 85, 98	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	VAL	4.4
1	A	166	PHE	4.0
1	B	215	ALA	4.0
1	A	211	ARG	4.0
1	B	173	GLY	3.7
1	B	211	ARG	3.6
1	A	172	ALA	3.6
1	A	329	ILE	3.4
1	B	17	ILE	3.4
1	B	258	GLY	3.4
1	A	196	GLY	3.3
1	A	165	ALA	3.2
1	B	363	ARG	3.1
1	A	206	GLU	3.1
1	B	29	ILE	3.1
1	A	304	GLU	3.1
1	B	204	ILE	3.0
1	A	363	ARG	2.9
1	A	16	VAL	2.9
1	B	18	CYS	2.7
1	B	154	ILE	2.7
1	B	253	ALA	2.7
1	A	173	GLY	2.7
1	B	257	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	27	ALA	2.6
1	B	218	ALA	2.6
1	A	328	ASN	2.6
1	A	207	GLU	2.6
1	A	231	ALA	2.5
1	A	248	ILE	2.5
1	A	272	LEU	2.5
1	B	231	ALA	2.5
1	B	207	GLU	2.5
1	B	214	ASP	2.5
1	B	227	TYR	2.5
1	A	257	ALA	2.5
1	B	220	ALA	2.5
1	A	201	ILE	2.5
1	B	205	ASN	2.5
1	B	252	LYS	2.4
1	A	204	ILE	2.4
1	A	237	CYS	2.4
1	B	28	ILE	2.4
1	B	246	GLU	2.4
1	A	214	ASP	2.3
1	B	88	LYS	2.3
1	B	196	GLY	2.3
1	B	46	TRP	2.3
1	A	258	GLY	2.3
1	A	251	LEU	2.3
1	A	49	ALA	2.2
1	A	215	ALA	2.2
1	A	303	ARG	2.2
1	B	181	VAL	2.2
1	A	314	TYR	2.2
1	A	17	ILE	2.2
1	A	15	LEU	2.2
1	A	236	PRO	2.1
1	A	275	GLU	2.1
1	B	15	LEU	2.1
1	A	212	ALA	2.1
1	A	216	PHE	2.1
1	B	199	LEU	2.1
1	A	230	GLU	2.1
1	B	163	LYS	2.0
1	A	278	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	254	LYS	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.