



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 AM UTC

PDB ID : 3VPX / pdb_00003vpX
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

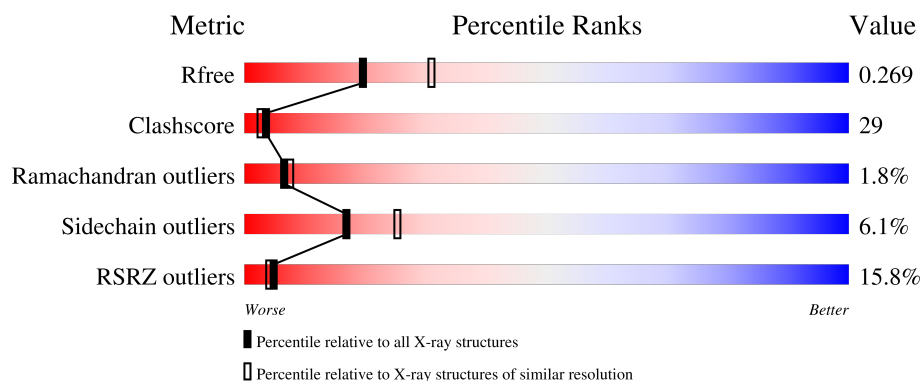
1 Overall quality at a glance

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	15% 52% 40% 6%
1	B	364	16% 52% 41% 5%

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, α , β , γ	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) 96.6 (31.78-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.63 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.290 0.267 , 0.269	Depositor DCC
R_{free} test set	1755 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5517	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	2/2757 (0.1%)	0.96	9/3729 (0.2%)
1	B	0.47	0/2771	0.98	12/3748 (0.3%)
All	All	0.48	2/5528 (0.0%)	0.97	21/7477 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	C-N	-9.35	1.20	1.33
1	A	52	GLU	C-N	-6.89	1.24	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLU	N-CA-C	-8.37	102.66	113.12
1	B	326	ARG	N-CA-C	-7.73	104.46	114.04
1	A	283	ASP	N-CA-C	6.87	119.40	111.02
1	B	90	ASP	N-CA-C	6.72	120.74	112.54
1	A	106	LEU	N-CA-C	-6.66	104.78	113.17
1	B	104	GLU	N-CA-C	-6.65	104.03	111.28
1	B	171	LEU	N-CA-C	-6.51	105.44	113.19
1	A	136	THR	CB-CA-C	-6.50	106.27	114.40
1	B	301	TYR	N-CA-C	6.45	119.33	110.24
1	B	353	PHE	N-CA-C	6.38	119.52	109.96
1	B	327	ASP	N-CA-C	-6.04	104.02	113.02
1	B	255	VAL	N-CA-C	5.92	118.50	108.86
1	B	253	ALA	N-CA-C	-5.83	97.82	108.02
1	A	97	ARG	N-CA-C	-5.75	104.92	111.14
1	B	107	ASN	N-CA-C	5.74	119.11	111.30
1	A	327	ASP	N-CA-C	-5.65	105.73	113.30
1	A	14	GLN	N-CA-C	5.51	117.56	109.24
1	A	353	PHE	N-CA-C	5.50	118.21	110.23
1	B	152	TYR	N-CA-C	-5.33	106.04	112.54
1	B	121	ALA	N-CA-C	-5.22	105.67	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	VAL	N-CA-C	5.11	115.71	107.73

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	2718	0	2680	155	0
1	B	2732	0	2693	167	0
2	A	37	0	0	1	0
2	B	30	0	0	1	0
All	All	5517	0	5373	319	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 29.

All (319) 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	1.02
1:B:154:ILE:HD11	1:B:188:LEU:HD13	1.44	0.98
1:B:158:MET:HE1	1:B:192:LEU:HD21	1.50	0.93
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:158:MET:HE3	1:B:171:LEU:HD13	1.52	0.90
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:PHE:CE2	1:A:236:PRO:HG3	2.17	0.80
1:A:248:ILE:HB	1:A:249:PRO:HD3	1.62	0.80
1:A:316:VAL:HG23	1:A:338:MET:HE1	1.65	0.78
1:A:363:ARG:H	1:A:363:ARG:HD2	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:B:200:ILE:C	1:B:200:ILE:HD13	2.17	0.70
1:A:50:SER:OG	1:A:53:GLU:HB2	1.90	0.70
1:B:162:ALA:C	1:B:164:GLU:H	1.97	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ALA:HB2	1:B:279:VAL:HG21	1.78	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:158:MET:HE3	1:B:171:LEU:CD1	2.28	0.64
1:B:81:THR:HG21	1:B:99:PHE:CZ	2.32	0.64
1:A:168:ASP:OD2	1:A:170:SER:HB3	1.99	0.63
1:B:43:THR:HG21	1:B:99:PHE:CE2	2.31	0.63
1:B:155:TYR:O	1:B:159:LYS:HG3	1.97	0.63
1:B:162:ALA:C	1:B:164:GLU:N	2.53	0.63
1:A:1:MET:N	1:A:52:GLU:OE2	2.31	0.63
1:A:44:ARG:HD2	1:A:116:VAL:CG2	2.29	0.63
1:B:323:ILE:HD12	1:B:338:MET:HB2	1.79	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:114:GLU:HA	1:B:118:THR:HG21	1.80	0.62
1:B:162:ALA:O	1:B:164:GLU:N	2.33	0.62
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:316:VAL:CG2	1:A:338:MET:HE1	2.31	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:A:202:THR:HG22	1:A:203:ASP:H	1.65	0.60
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:A:162:ALA:HB2	1:A:171:LEU:HD21	1.85	0.59
1:B:166:PHE:CZ	1:B:232:ASP:HB2	2.38	0.59
1:B:255:VAL:HG13	1:B:279:VAL:HG23	1.85	0.59
1:A:199:LEU:N	1:A:199:LEU:HD12	2.18	0.59
1:B:228:SER:HB3	1:B:250:GLN:HE21	1.68	0.59
1:A:181:VAL:HG12	1:A:181:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:HIS:O	1:A:273:ILE:HG23	2.02	0.58
1:B:204:ILE:HD12	1:B:204:ILE:N	2.14	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:287:ASN:C	1:A:287:ASN:HD22	2.14	0.56
1:A:28:ILE:HB	1:A:82:VAL:HG22	1.86	0.56
1:B:275:GLU:OE1	1:B:275:GLU:HA	2.04	0.56
1:B:280:TYR:O	1:B:282:PRO:HD3	2.06	0.55
1:B:312:GLY:O	1:B:316:VAL:HG23	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:A:13:GLU:OE2	1:A:33:ASP:HA	2.08	0.53
1:B:145:ASN:ND2	1:B:145:ASN:O	2.41	0.53
1:A:162:ALA:HB2	1:A:171:LEU:CD2	2.38	0.53
1:B:43:THR:HA	1:B:81:THR:O	2.08	0.53
1:B:57:ASP:OD1	1:B:60:ARG:NH1	2.41	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
1:B:255:VAL:HG12	1:B:256:ILE:N	2.24	0.53
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:161:ALA:O	1:B:164:GLU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:O	1:B:213:VAL:HG22	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:B:86:ASN:C	1:B:86:ASN:HD22	2.19	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:84:ILE:HG13	1:B:84:ILE:O	2.11	0.51
1:B:154:ILE:HD13	1:B:155:TYR:H	1.76	0.51
1:B:163:LYS:HA	1:B:167:GLY:C	2.36	0.50
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:158:MET:HE1	1:B:192:LEU:CD2	2.32	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:200:ILE:C	1:B:200:ILE:CD1	2.86	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:A:293:ASN:HD22	1:A:306:ALA:HB1	1.78	0.49
1:B:200:ILE:HG12	1:B:219:THR:O	2.13	0.49
1:B:105:GLY:C	1:B:107:ASN:H	2.21	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:94:GLU:CD	1:A:94:GLU:H	2.21	0.48
1:A:284:TYR:HA	1:A:287:ASN:HD21	1.78	0.48
1:B:194:GLU:C	1:B:196:GLY:H	2.21	0.48
1:B:195:GLU:HG2	1:B:195:GLU:O	2.12	0.48
1:A:44:ARG:CD	1:A:115:ASP:OD2	2.61	0.48
1:B:288:SER:C	1:B:290:GLY:H	2.22	0.48
1:B:181:VAL:HG23	1:B:203:ASP:HB2	1.95	0.48
1:B:221:VAL:CG1	1:B:225:GLU:HB2	2.44	0.48
1:A:44:ARG:HG3	1:A:116:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2:GLU:HG2	1:A:5:LYS:HB2	1.97	0.47
1:A:149:VAL:HG11	1:A:293:ASN:ND2	2.30	0.47
1:B:227:TYR:O	1:B:251:LEU:HD23	2.15	0.47
1:B:314:TYR:CD1	1:B:314:TYR:C	2.93	0.47
1:B:240:GLY:C	1:B:242:ILE:H	2.22	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:A:40:LEU:HD23	1:A:41:GLY:N	2.29	0.46
1:B:209:VAL:O	1:B:213:VAL:HG13	2.15	0.46
1:A:323:ILE:HB	1:A:334:ALA:HB1	1.97	0.46
1:B:151:ALA:O	1:B:154:ILE:CD1	2.56	0.46
1:A:120:GLU:OE1	1:A:137:SER:O	2.33	0.46
1:B:170:SER:C	1:B:172:ALA:H	2.22	0.46
1:B:200:ILE:HD13	1:B:201:ILE:N	2.30	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:201:ILE:CD1	1:B:209:VAL:HG13	2.45	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:242:ILE:N	1:A:242:ILE:HD13	2.31	0.46
1:B:165:ALA:HB2	1:B:279:VAL:CG2	2.45	0.46
1:B:213:VAL:HG23	1:B:214:ASP:N	2.31	0.46
1:B:221:VAL:HG12	1:B:225:GLU:HB2	1.97	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: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
1:B:118:THR:HG23	1:B:123:MET:HE3	1.98	0.45
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:B:94:GLU:H	1:B:94:GLU:CD	2.25	0.45
1:A:285:VAL:O	1:A:288:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:210:GLN:O	1:A:211:ARG:C	2.60	0.45
1:B:319:LYS:HB3	1:B:338:MET:HE1	1.99	0.45
1:B:359:SER:C	1:B:361:LEU:H	2.23	0.45
1:A:296:ASP:CG	1:A:305:ARG:HH21	2.25	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: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:A:200:ILE:HD13	1:A:229:GLN:HB3	2.00	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: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:B:288:SER:C	1:B:290:GLY:N	2.71	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: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:B:319:LYS:HB3	1:B:338:MET:CE	2.48	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:B:309:ARG:HD3	1:B:309:ARG:C	2.42	0.44
1:A:28:ILE:HB	1:A:82:VAL:CG2	2.48	0.44
1:A:114:GLU:HG3	1:A:123:MET:CG	2.48	0.44
1:A:172:ALA:HA	1:A:196:GLY:O	2.18	0.44
1:B:86:ASN:HD22	1:B:87:PRO:CD	2.31	0.44
1:B:293:ASN:HD22	1:B:306:ALA:HB1	1.83	0.44
1:A:221:VAL:HG11	1:A:229:GLN:CD	2.43	0.44
1:A:288:SER:O	1:A:290:GLY:N	2.51	0.43
1:B:43:THR:CG2	1:B:112:THR:OG1	2.66	0.43
1:B:161:ALA:HB1	1:B:255:VAL:CG1	2.48	0.43
1:B:305:ARG:O	1:B:309:ARG:HB2	2.17	0.43
1:A:205:ASN:HD22	1:A:208:ALA:CB	2.31	0.43
1:B:279:VAL:HG23	1:B:279:VAL:O	2.18	0.43
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.91	0.43
1:B:205:ASN:ND2	1:B:208:ALA:HB2	2.32	0.43
1:B:254:LYS:O	1:B:279:VAL:HG22	2.19	0.43
1:B:323:ILE:CD1	1:B:338:MET:HB2	2.46	0.43
1:A:21:LYS:HB2	1:B:11:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:HB3	1:A:242:ILE:HG13	2.01	0.43
1:A:201:ILE:HD12	1:A:212:ALA:HB3	2.00	0.43
1:B:114:GLU:OE2	1:B:120:GLU:HA	2.19	0.43
1:B:207:GLU:OE2	1:B:207:GLU:HA	2.18	0.43
1:B:146:PRO:O	1:B:149:VAL:N	2.49	0.43
1:B:205:ASN:HB3	1:B:208:ALA:HB3	2.00	0.43
1:A:50:SER:HG	1:A:53:GLU:HB2	1.83	0.43
1:B:40:LEU:C	1:B:40:LEU:HD23	2.43	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:232:ASP:O	1:B:233:ILE:HG13	2.19	0.43
1:B:50:SER:O	1:B:53:GLU:HB3	2.19	0.42
1:B:170:SER:C	1:B:172:ALA:N	2.78	0.42
1:A:159:LYS:HG3	1:A:169:ASP:O	2.19	0.42
1:A:271:ASP:HB2	1:A:272:LEU:HD22	2.01	0.42
1:A:4:PHE:HB2	1:B:51:GLU:OE2	2.19	0.42
1:A:341:GLU:O	1:A:345:ARG:HG3	2.19	0.42
1:B:302:ASN:C	1:B:302:ASN:ND2	2.77	0.42
1:B:302:ASN:C	1:B:302:ASN:HD22	2.26	0.42
1:A:200:ILE:HG21	1:A:229:GLN:HG3	2.01	0.42
1:B:46:TRP:CD1	1:B:47:THR:H	2.38	0.42
1:B:163:LYS:O	1:B:163:LYS:HG3	2.20	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:A:145:ASN:N	1:A:145:ASN:ND2	2.65	0.42
1:B:149:VAL:HA	1:B:307:LEU:CD2	2.49	0.42
1:B:240:GLY:C	1:B:242:ILE:N	2.76	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:90:ASP:OD2	1:A:90:ASP:N	2.49	0.41
1:A:145:ASN:ND2	1:A:145:ASN:O	2.53	0.41
1:A:287:ASN:C	1:A:287:ASN:ND2	2.78	0.41
1:A:288:SER:C	1:A:290:GLY:N	2.77	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:146:PRO:O	1:B:147:SER:C	2.63	0.41
1:A:249:PRO:O	1:A:250:GLN:C	2.63	0.41
1:B:228:SER:HB3	1:B:250:GLN:NE2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HB2	1:A:80:LYS:HG2	2.03	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: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:A:153:GLY:HA2	1:A:310:VAL:CG1	2.52	0.40
1:A:158:MET:HE2	1:A:233:ILE:HG21	2.03	0.40
1:A:186:TYR:O	1:A:189:CYS:HB2	2.21	0.40
1:A:316:VAL:HG23	1:A:338:MET:CE	2.44	0.40
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.85	0.40
1:B:194:GLU:C	1:B:196:GLY:N	2.79	0.40
1:B:255:VAL:HG22	1:B:279:VAL:HG21	2.02	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:B:359:SER:C	1:B:361:LEU:N	2.77	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%)	6	6
1	B	355/364 (98%)	305 (86%)	44 (12%)	6 (2%)	7	8
All	All	707/728 (97%)	614 (87%)	80 (11%)	13 (2%)	6	7

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASP

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Mol	Chain	Res	Type
1	A	229	GLN
1	B	174	LYS
1	B	203	ASP
1	A	90	ASP
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%)	17	25
1	B	278/281 (99%)	261 (94%)	17 (6%)	17	25
All	All	556/562 (99%)	522 (94%)	34 (6%)	17	25

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	44	ARG
1	A	66	THR
1	A	97	ARG
1	A	128	LEU
1	A	145	ASN
1	A	150	THR
1	A	164	GLU
1	A	199	LEU
1	A	226	ILE
1	A	242	ILE

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Mol	Chain	Res	Type
1	A	287	ASN
1	A	288	SER
1	A	310	VAL
1	A	316	VAL
1	A	359	SER
1	A	363	ARG
1	B	43	THR
1	B	44	ARG
1	B	66	THR
1	B	84	ILE
1	B	112	THR
1	B	118	THR
1	B	128	LEU
1	B	133	VAL
1	B	145	ASN
1	B	150	THR
1	B	154	ILE
1	B	194	GLU
1	B	200	ILE
1	B	223	ILE
1	B	250	GLN
1	B	272	LEU
1	B	317	ILE

Sometimes 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	145	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	205	ASN
1	B	250	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	356/364 (97%)	0.93	55 (15%) 5 4	23, 52, 87, 98	0
1	B	359/364 (98%)	0.96	58 (16%) 4 3	23, 51, 82, 94	0
All	All	715/728 (98%)	0.94	113 (15%) 5 4	23, 51, 85, 98	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	ALA	4.9
1	B	204	ILE	4.9
1	A	202	THR	4.7
1	A	304	GLU	4.6
1	B	215	ALA	4.5
1	A	223	ILE	4.5
1	B	227	TYR	4.4
1	B	231	ALA	4.3
1	A	200	ILE	4.0
1	B	171	LEU	4.0
1	A	219	THR	3.9
1	A	278	ILE	3.8
1	B	219	THR	3.7
1	A	173	GLY	3.6
1	A	166	PHE	3.6
1	B	250	GLN	3.5
1	B	52	GLU	3.5
1	A	52	GLU	3.4
1	B	252	LYS	3.4
1	B	246	GLU	3.3
1	A	220	ALA	3.2
1	A	231	ALA	3.2
1	A	197	ALA	3.2
1	A	199	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	137	SER	3.1
1	B	199	LEU	3.1
1	A	227	TYR	3.0
1	A	272	LEU	3.0
1	A	329	ILE	3.0
1	A	211	ARG	3.0
1	A	251	LEU	3.0
1	A	216	PHE	3.0
1	A	171	LEU	3.0
1	A	248	ILE	2.9
1	B	165	ALA	2.9
1	A	363	ARG	2.9
1	A	167	GLY	2.9
1	B	226	ILE	2.9
1	B	251	LEU	2.9
1	A	165	ALA	2.8
1	B	317	ILE	2.8
1	B	213	VAL	2.8
1	B	216	PHE	2.8
1	B	241	ALA	2.8
1	A	210	GLN	2.8
1	B	200	ILE	2.8
1	B	228	SER	2.8
1	A	214	ASP	2.8
1	A	212	ALA	2.7
1	B	166	PHE	2.7
1	A	198	LYS	2.7
1	B	254	LYS	2.7
1	B	172	ALA	2.7
1	A	273	ILE	2.7
1	B	149	VAL	2.6
1	A	196	GLY	2.6
1	A	204	ILE	2.6
1	A	228	SER	2.6
1	B	223	ILE	2.6
1	B	233	ILE	2.6
1	B	255	VAL	2.6
1	A	175	THR	2.5
1	B	175	THR	2.5
1	B	205	ASN	2.5
1	B	316	VAL	2.5
1	A	49	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	2.5
1	A	201	ILE	2.5
1	A	252	LYS	2.5
1	B	193	HIS	2.4
1	B	206	GLU	2.4
1	B	220	ALA	2.4
1	B	203	ASP	2.4
1	B	140	ALA	2.4
1	B	197	ALA	2.4
1	A	254	LYS	2.4
1	A	209	VAL	2.4
1	A	224	ASN	2.4
1	B	299	ASP	2.3
1	A	208	ALA	2.3
1	A	217	GLY	2.3
1	B	352	THR	2.3
1	A	250	GLN	2.3
1	B	176	VAL	2.3
1	A	145	ASN	2.3
1	B	162	ALA	2.3
1	B	248	ILE	2.3
1	B	218	ALA	2.2
1	A	299	ASP	2.2
1	A	246	GLU	2.2
1	B	145	ASN	2.2
1	B	257	ALA	2.2
1	B	300	GLY	2.2
1	B	169	ASP	2.2
1	B	191	TYR	2.2
1	A	257	ALA	2.1
1	B	154	ILE	2.1
1	A	46	TRP	2.1
1	B	247	THR	2.1
1	B	201	ILE	2.1
1	A	314	TYR	2.1
1	B	268	ARG	2.1
1	A	226	ILE	2.1
1	A	230	GLU	2.1
1	B	186	TYR	2.1
1	B	221	VAL	2.1
1	A	328	ASN	2.1
1	A	247	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	221	VAL	2.0
1	B	345	ARG	2.0
1	B	363	ARG	2.0
1	B	163	LYS	2.0
1	B	207	GLU	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 oligosaccharides 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.