



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:40 PM EDT

PDB ID : 3H8E / pdb_00003h8e
Title : Low pH native structure of leucine aminopeptidase from *Pseudomonas putida*
Authors : Kale, A.; Dijkstra, B.W.; Sonke, T.; Thunnissen, A.M.W.H.
Deposited on : 2009-04-29
Resolution : 2.75 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

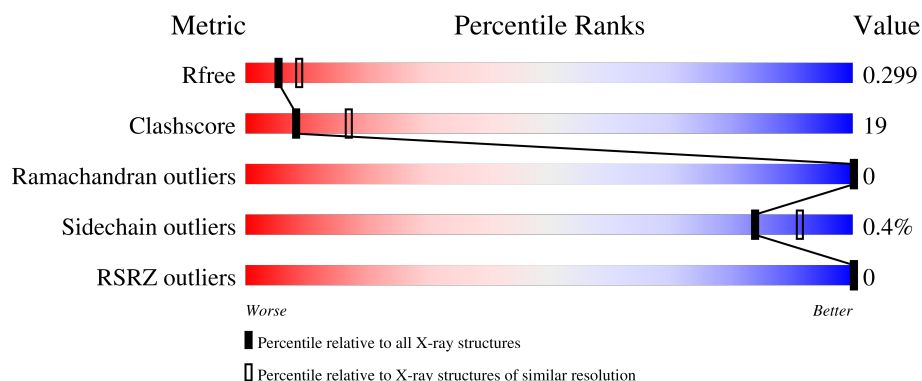
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	497	 74% 19% • 5%
1	B	497	 71% 21% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7006 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.

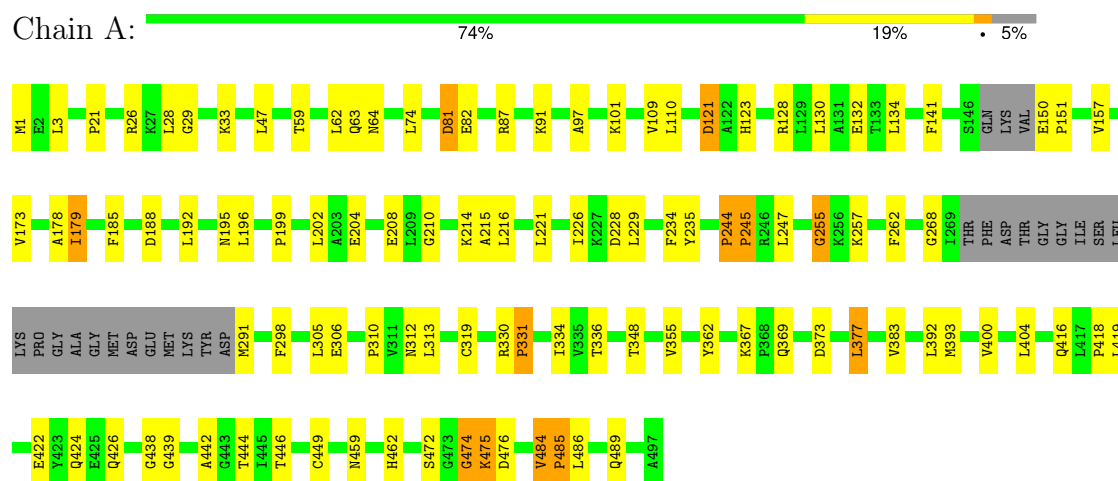
- Molecule 1 is a protein called Cytosol aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3503	2212	616	659	16			
1	B	473	Total	C	N	O	S	0	0	0
			3503	2212	616	659	16			

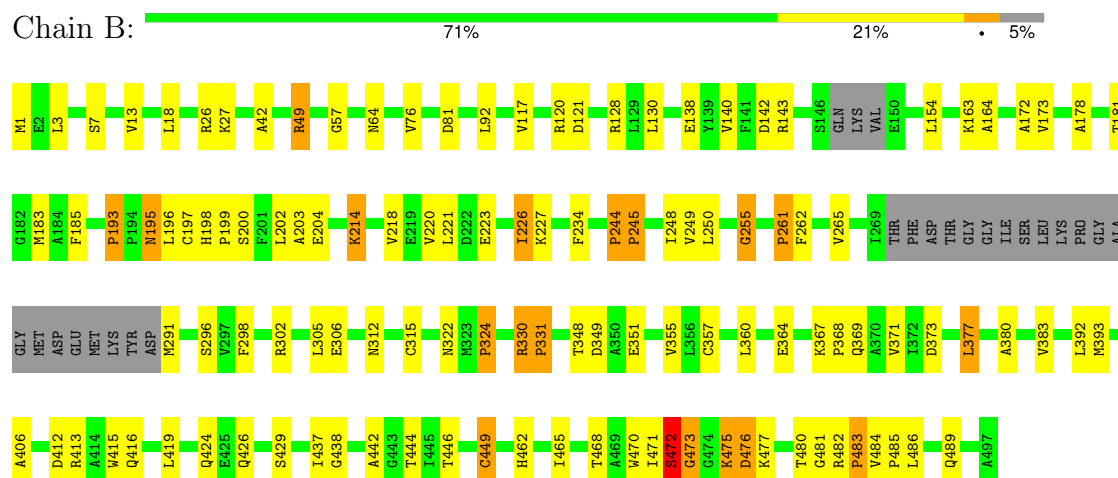
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Cytosol aminopeptidase



• Molecule 1: Cytosol aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	116.95Å 116.95Å 137.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.00 – 2.75 58.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.00-2.75) 100.0 (58.00-2.75)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.267 0.290 , 0.299	Depositor DCC
R_{free} test set	1399 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 14.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-h-k,-l	Depositor
Outliers	0 of 27831 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7006	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	1.69	24/3553 (0.7%)	1.47	17/4805 (0.4%)
1	B	1.64	26/3553 (0.7%)	1.45	23/4805 (0.5%)
All	All	1.67	50/7106 (0.7%)	1.46	40/9610 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	PRO	N-CD	-10.48	1.33	1.47
1	B	220	VAL	C-O	8.73	1.33	1.24
1	B	305	LEU	C-O	8.08	1.33	1.24
1	B	42	ALA	C-O	8.03	1.33	1.24
1	B	172	ALA	N-CA	7.36	1.55	1.46
1	A	484	VAL	CA-CB	-7.33	1.49	1.53
1	B	245	PRO	N-CD	-7.27	1.37	1.47
1	B	324	PRO	N-CD	-7.07	1.37	1.47
1	B	255	GLY	N-CA	7.06	1.51	1.44
1	A	62	LEU	CA-C	-7.05	1.44	1.52
1	A	216	LEU	N-CA	6.86	1.54	1.46
1	B	13	VAL	CA-CB	6.54	1.62	1.54
1	A	229	LEU	N-CA	6.28	1.54	1.46
1	A	151	PRO	N-CD	-6.28	1.39	1.47
1	A	439	GLY	N-CA	6.26	1.53	1.44
1	B	204	GLU	N-CA	6.25	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	GLY	N-CA	6.04	1.54	1.45
1	B	360	LEU	C-O	6.01	1.31	1.24
1	B	380	ALA	CA-CB	5.99	1.63	1.53
1	A	438	GLY	N-CA	5.91	1.53	1.45
1	A	228	ASP	C-O	5.86	1.31	1.24
1	A	235	TYR	CD1-CE1	5.70	1.55	1.38
1	A	334	ILE	N-CA	5.63	1.52	1.46
1	A	121	ASP	N-CA	5.62	1.53	1.46
1	A	255	GLY	C-O	-5.62	1.18	1.23
1	A	179	ILE	CA-CB	-5.60	1.47	1.54
1	A	257	LYS	CA-CB	5.57	1.62	1.53
1	B	367	LYS	CA-CB	5.52	1.57	1.52
1	A	313	LEU	CA-C	-5.51	1.46	1.52
1	A	123	HIS	CA-CB	-5.50	1.44	1.54
1	A	310	PRO	CA-C	-5.40	1.48	1.53
1	B	406	ALA	CA-C	5.40	1.59	1.52
1	A	121	ASP	C-O	5.35	1.30	1.23
1	B	203	ALA	N-CA	5.34	1.52	1.46
1	B	449	CYS	C-O	5.33	1.30	1.24
1	B	315	CYS	N-CA	5.31	1.52	1.46
1	B	140	VAL	CA-CB	5.29	1.62	1.54
1	B	322	ASN	N-CA	5.28	1.53	1.46
1	A	21	PRO	C-O	5.21	1.29	1.23
1	A	459	ASN	N-CA	5.21	1.52	1.46
1	B	371	VAL	N-CA	5.21	1.53	1.46
1	B	227	LYS	CA-C	5.21	1.59	1.52
1	B	226	ILE	CA-CB	5.19	1.60	1.54
1	B	142	ASP	N-CA	5.17	1.52	1.46
1	B	195	ASN	CG-OD1	5.17	1.33	1.23
1	A	81	ASP	N-CA	5.14	1.52	1.46
1	A	362	TYR	C-O	5.11	1.30	1.24
1	B	429	SER	CA-C	-5.04	1.48	1.52
1	A	305	LEU	N-CA	5.04	1.52	1.46
1	B	18	LEU	C-O	-5.01	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	PRO	CA-N-CD	-9.99	98.02	112.00
1	A	151	PRO	CA-N-CD	-8.84	99.62	112.00
1	B	244	PRO	CA-N-CD	-8.53	100.06	112.00
1	B	261	PRO	CA-N-CD	-8.45	100.17	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	PRO	CA-N-CD	-8.36	100.29	112.00
1	B	193	PRO	CA-N-CD	-8.33	100.33	112.00
1	B	483	PRO	CA-N-CD	-8.23	100.48	112.00
1	B	199	PRO	CA-N-CD	-8.15	100.59	112.00
1	A	245	PRO	CA-N-CD	-8.13	100.62	112.00
1	A	485	PRO	CA-N-CD	-8.11	100.64	112.00
1	B	331	PRO	CA-N-CD	-8.04	100.74	112.00
1	A	150	GLU	CA-C-N	8.01	128.07	119.90
1	A	150	GLU	C-N-CA	8.01	128.07	119.90
1	B	472	SER	N-CA-C	7.98	121.66	108.49
1	A	244	PRO	CA-N-CD	-7.83	101.04	112.00
1	B	245	PRO	CA-N-CD	-7.76	101.14	112.00
1	A	331	PRO	CA-N-CD	-7.29	101.80	112.00
1	A	64	ASN	CB-CA-C	-7.09	99.94	110.16
1	B	324	PRO	CA-N-CD	-6.94	102.28	112.00
1	A	474	GLY	N-CA-C	-6.80	101.26	112.83
1	B	367	LYS	O-C-N	-6.06	118.74	121.53
1	B	484	VAL	CB-CA-C	-5.89	108.11	114.35
1	B	214	LYS	N-CA-C	5.88	117.69	111.28
1	A	214	LYS	N-CA-C	5.78	118.32	111.33
1	A	472	SER	N-CA-C	5.61	118.33	111.82
1	B	475	LYS	N-CA-C	5.57	120.08	113.28
1	B	305	LEU	CA-C-O	-5.56	114.66	120.55
1	B	367	LYS	CA-C-O	5.51	124.67	120.26
1	B	357	CYS	CA-C-O	-5.36	114.74	120.42
1	B	364	GLU	CA-C-O	-5.33	114.23	120.20
1	B	49	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	367	LYS	CA-C-O	5.25	124.52	120.48
1	B	64	ASN	CB-CA-C	-5.22	102.81	110.06
1	B	265	VAL	CA-C-N	-5.11	117.84	122.80
1	B	265	VAL	C-N-CA	-5.11	117.84	122.80
1	B	143	ARG	N-CA-C	5.11	118.61	112.38
1	A	305	LEU	CA-C-O	-5.10	115.01	120.42
1	B	437	ILE	O-C-N	5.10	128.70	123.04
1	A	215	ALA	N-CA-C	-5.09	106.91	113.02
1	A	210	GLY	O-C-N	5.08	127.16	122.13

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	474	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	475	LYS	Peptide
1	B	472	SER	Peptide
1	B	473	GLY	Peptide
1	B	476	ASP	Peptide

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	3503	0	3600	127	11
1	B	3503	0	3600	153	12
All	All	7006	0	7200	273	12

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 19.

All (273) 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:226:ILE:HD13	1:A:234:PHE:CE2	1.28	1.65
1:B:226:ILE:HD13	1:B:234:PHE:CE2	1.10	1.62
1:B:226:ILE:CD1	1:B:234:PHE:HE2	1.13	1.52
1:A:185:PHE:CE2	1:A:298:PHE:HB3	1.44	1.51
1:B:473:GLY:CA	1:B:477:LYS:HG3	1.38	1.49
1:A:226:ILE:CD1	1:A:234:PHE:HE2	1.28	1.45
1:B:185:PHE:CE2	1:B:298:PHE:HB3	1.54	1.40
1:A:185:PHE:HE2	1:A:298:PHE:CB	1.44	1.29
1:B:226:ILE:HG21	1:B:234:PHE:CD2	1.68	1.28
1:A:195:ASN:OD1	1:A:196:LEU:HG	1.34	1.25
1:A:1:MET:HE1	1:A:134:LEU:CG	1.68	1.24
1:A:1:MET:CE	1:A:134:LEU:HG	1.71	1.21
1:A:400:VAL:O	1:A:404:LEU:HD13	1.37	1.20
1:A:262:PHE:CZ	1:A:369:GLN:NE2	2.09	1.20
1:B:185:PHE:HE2	1:B:298:PHE:CB	1.54	1.19
1:A:188:ASP:O	1:A:192:LEU:HD23	1.37	1.18
1:B:473:GLY:CA	1:B:477:LYS:CG	2.21	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:CG2	1:B:234:PHE:HD2	1.57	1.16
1:A:226:ILE:HG21	1:A:234:PHE:HD2	1.08	1.16
1:B:424:GLN:NE2	1:B:449:CYS:SG	2.19	1.15
1:B:202:LEU:HD11	1:B:291:MET:CE	1.76	1.14
1:B:226:ILE:CD1	1:B:234:PHE:CE2	1.98	1.13
1:B:296:SER:HB2	1:B:483:PRO:HB2	1.26	1.13
1:B:471:ILE:HG22	1:B:473:GLY:O	1.48	1.12
1:B:473:GLY:HA2	1:B:477:LYS:CG	1.79	1.11
1:B:473:GLY:HA2	1:B:477:LYS:HG3	1.18	1.11
1:B:3:LEU:HD23	1:B:173:VAL:HG13	1.15	1.11
1:B:202:LEU:HD21	1:B:291:MET:HE1	1.21	1.10
1:B:468:THR:HB	1:B:482:ARG:HD3	1.35	1.08
1:B:262:PHE:CZ	1:B:369:GLN:NE2	2.23	1.06
1:A:226:ILE:HG21	1:A:234:PHE:CD2	1.89	1.05
1:B:473:GLY:HA3	1:B:477:LYS:HG3	1.11	1.04
1:A:226:ILE:CG2	1:A:234:PHE:HD2	1.71	1.04
1:A:331:PRO:HD3	1:A:348:THR:HG23	1.37	1.03
1:B:473:GLY:HA3	1:B:477:LYS:CG	1.82	1.03
1:B:331:PRO:HD3	1:B:348:THR:HG23	1.38	1.02
1:B:424:GLN:HE22	1:B:449:CYS:CB	1.72	1.02
1:B:226:ILE:HG21	1:B:234:PHE:HD2	0.89	1.02
1:A:226:ILE:CD1	1:A:234:PHE:CE2	2.15	1.01
1:A:3:LEU:HD22	1:A:173:VAL:CG1	1.91	1.00
1:B:202:LEU:HD11	1:B:291:MET:HE3	1.42	1.00
1:B:183:MET:HE3	1:B:481:GLY:HA3	1.43	0.99
1:A:26:ARG:HD3	1:A:47:LEU:O	1.63	0.99
1:A:392:LEU:HD23	1:A:404:LEU:HD11	1.42	0.99
1:B:202:LEU:CD2	1:B:291:MET:HE1	1.92	0.98
1:B:183:MET:CE	1:B:481:GLY:HA3	1.94	0.97
1:B:226:ILE:CG2	1:B:234:PHE:CD2	2.38	0.97
1:A:424:GLN:NE2	1:A:449:CYS:SG	2.38	0.96
1:A:373:ASP:OD1	1:A:462:HIS:HA	1.65	0.95
1:B:471:ILE:CG2	1:B:473:GLY:O	2.14	0.94
1:B:393:MET:SD	1:B:419:LEU:HD21	2.07	0.93
1:B:128:ARG:HH12	1:B:489:GLN:HE22	1.15	0.93
1:B:3:LEU:HD23	1:B:173:VAL:CG1	1.99	0.92
1:A:1:MET:HE1	1:A:134:LEU:HG	0.92	0.92
1:A:3:LEU:CD2	1:A:173:VAL:HG21	1.98	0.92
1:B:324:PRO:HD2	1:B:324:PRO:O	1.67	0.91
1:A:28:LEU:O	1:A:33:LYS:HE2	1.70	0.91
1:B:373:ASP:OD1	1:B:462:HIS:HA	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:CD2	1:A:173:VAL:CG2	2.50	0.89
1:A:377:LEU:HD12	1:A:377:LEU:O	1.72	0.89
1:B:377:LEU:O	1:B:377:LEU:HD12	1.72	0.88
1:A:400:VAL:O	1:A:404:LEU:CD1	2.21	0.87
1:B:424:GLN:NE2	1:B:449:CYS:CB	2.36	0.87
1:A:393:MET:SD	1:A:419:LEU:HD21	2.16	0.85
1:A:392:LEU:CD2	1:A:404:LEU:HD11	2.05	0.85
1:A:128:ARG:HH22	1:A:489:GLN:HE22	1.19	0.85
1:A:392:LEU:CD2	1:A:404:LEU:CD1	2.55	0.85
1:B:261:PRO:HD2	1:B:368:PRO:HA	1.57	0.84
1:B:202:LEU:CD1	1:B:291:MET:CE	2.55	0.84
1:B:76:VAL:HG22	1:B:92:LEU:HD21	1.60	0.83
1:A:392:LEU:HD23	1:A:404:LEU:CD1	2.09	0.83
1:B:248:ILE:HG22	1:B:250:LEU:HD11	1.60	0.82
1:B:248:ILE:HG22	1:B:250:LEU:CD1	2.10	0.82
1:B:412:ASP:OD2	1:B:482:ARG:O	1.98	0.82
1:B:296:SER:CB	1:B:483:PRO:HB2	2.07	0.81
1:A:3:LEU:HD22	1:A:173:VAL:CG2	2.10	0.80
1:B:76:VAL:CG2	1:B:92:LEU:HD21	2.11	0.80
1:A:3:LEU:HD21	1:A:173:VAL:HG21	1.63	0.80
1:B:424:GLN:NE2	1:B:449:CYS:HB3	1.97	0.80
1:B:193:PRO:HD2	1:B:193:PRO:O	1.81	0.80
1:B:178:ALA:HA	1:B:306:GLU:OE1	1.82	0.79
1:B:202:LEU:HD21	1:B:291:MET:CE	2.09	0.78
1:B:424:GLN:HE22	1:B:449:CYS:HB3	1.47	0.78
1:B:202:LEU:CD1	1:B:291:MET:HE3	2.12	0.78
1:A:226:ILE:CG2	1:A:234:PHE:CD2	2.57	0.78
1:A:141:PHE:CZ	1:A:192:LEU:HD22	2.20	0.77
1:A:3:LEU:HD21	1:A:173:VAL:CG2	2.14	0.76
1:B:473:GLY:HA3	1:B:477:LYS:CD	2.14	0.76
1:A:3:LEU:HD22	1:A:173:VAL:HG11	1.67	0.75
1:B:331:PRO:HD3	1:B:348:THR:CG2	2.16	0.75
1:A:393:MET:HE3	1:A:462:HIS:HD2	1.52	0.75
1:A:195:ASN:OD1	1:A:196:LEU:N	2.20	0.75
1:B:183:MET:HE3	1:B:481:GLY:CA	2.17	0.74
1:B:296:SER:HB3	1:B:483:PRO:HG2	1.69	0.74
1:B:296:SER:HB2	1:B:483:PRO:CB	2.11	0.74
1:B:197:CYS:SG	1:B:291:MET:SD	2.85	0.74
1:A:3:LEU:HD22	1:A:173:VAL:HG13	1.70	0.73
1:A:110:LEU:HD12	1:A:110:LEU:N	2.03	0.73
1:A:244:PRO:HD2	1:A:244:PRO:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:PRO:HD2	1:B:244:PRO:O	1.89	0.72
1:B:195:ASN:OD1	1:B:196:LEU:HG	1.89	0.72
1:B:249:VAL:C	1:B:250:LEU:HD12	2.15	0.72
1:A:268:GLY:HA2	1:A:291:MET:HG3	1.70	0.71
1:A:331:PRO:HD3	1:A:348:THR:CG2	2.17	0.70
1:B:245:PRO:HD2	1:B:245:PRO:O	1.92	0.69
1:B:468:THR:HB	1:B:482:ARG:CD	2.18	0.69
1:B:202:LEU:HD11	1:B:291:MET:HE1	1.68	0.69
1:B:261:PRO:HD2	1:B:261:PRO:O	1.93	0.68
1:A:392:LEU:CD2	1:A:404:LEU:HD12	2.23	0.68
1:A:87:ARG:HG3	1:A:91:LYS:HE3	1.76	0.67
1:B:296:SER:CB	1:B:483:PRO:CB	2.70	0.67
1:A:110:LEU:HD13	1:A:157:VAL:HG13	1.76	0.67
1:A:178:ALA:HA	1:A:306:GLU:OE1	1.96	0.66
1:A:418:PRO:HD3	1:B:415:TRP:CE2	2.31	0.66
1:A:141:PHE:HZ	1:A:192:LEU:HD22	1.61	0.66
1:B:202:LEU:CD1	1:B:291:MET:HE1	2.24	0.66
1:B:472:SER:N	1:B:473:GLY:O	2.30	0.65
1:B:248:ILE:CG2	1:B:250:LEU:HD11	2.26	0.64
1:A:245:PRO:HD2	1:A:245:PRO:O	1.98	0.64
1:B:183:MET:HE2	1:B:481:GLY:HA3	1.79	0.64
1:A:383:VAL:O	1:B:442:ALA:HA	1.97	0.63
1:B:185:PHE:HE2	1:B:298:PHE:HB3	0.63	0.63
1:A:418:PRO:HD3	1:B:415:TRP:NE1	2.14	0.62
1:A:195:ASN:OD1	1:A:196:LEU:CG	2.28	0.62
1:A:110:LEU:N	1:A:110:LEU:CD1	2.62	0.61
1:B:473:GLY:HA2	1:B:477:LYS:HG2	1.76	0.61
1:B:202:LEU:CG	1:B:291:MET:HE1	2.30	0.61
1:B:473:GLY:CA	1:B:477:LYS:CD	2.75	0.61
1:B:324:PRO:O	1:B:324:PRO:CD	2.43	0.60
1:A:1:MET:HE1	1:A:134:LEU:CD2	2.29	0.60
1:B:473:GLY:HA3	1:B:477:LYS:HD2	1.84	0.60
1:B:262:PHE:HZ	1:B:369:GLN:NE2	1.95	0.60
1:B:226:ILE:HD11	1:B:234:PHE:CE2	2.29	0.59
1:A:404:LEU:HD12	1:A:404:LEU:N	2.18	0.58
1:B:226:ILE:HG21	1:B:234:PHE:CE2	2.33	0.58
1:A:110:LEU:CD1	1:A:157:VAL:HG13	2.34	0.58
1:B:226:ILE:HG23	1:B:234:PHE:CD2	2.33	0.58
1:A:255:GLY:H	1:A:312:ASN:ND2	2.01	0.58
1:B:57:GLY:N	1:B:92:LEU:HD23	2.19	0.58
1:B:226:ILE:HD13	1:B:234:PHE:CD2	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:CD2	1:A:173:VAL:HG22	2.31	0.58
1:B:226:ILE:CG1	1:B:234:PHE:CE2	2.84	0.58
1:A:422:GLU:CD	1:B:413:ARG:HH22	2.11	0.58
1:B:426:GLN:OE1	1:B:446:THR:HG21	2.05	0.56
1:A:393:MET:SD	1:A:419:LEU:CD2	2.91	0.56
1:B:27:LYS:NZ	1:B:81:ASP:OD2	2.38	0.56
1:B:480:THR:CB	1:B:482:ARG:HG3	2.36	0.56
1:B:128:ARG:NH1	1:B:489:GLN:HE22	1.97	0.56
1:B:481:GLY:O	1:B:485:PRO:HD3	2.06	0.56
1:B:76:VAL:CG2	1:B:92:LEU:CD2	2.81	0.56
1:A:26:ARG:HD2	1:A:47:LEU:HB3	1.88	0.55
1:B:473:GLY:CA	1:B:477:LYS:HD2	2.35	0.55
1:B:480:THR:HB	1:B:482:ARG:HG3	1.88	0.55
1:B:470:TRP:CD1	1:B:472:SER:HB3	2.42	0.55
1:B:261:PRO:CD	1:B:368:PRO:HA	2.32	0.55
1:A:418:PRO:HB3	1:B:415:TRP:CH2	2.42	0.55
1:B:470:TRP:NE1	1:B:472:SER:HB3	2.21	0.55
1:A:110:LEU:HD13	1:A:157:VAL:CG1	2.37	0.54
1:A:185:PHE:CE2	1:A:298:PHE:CG	2.95	0.54
1:A:262:PHE:CE2	1:A:369:GLN:NE2	2.71	0.54
1:B:3:LEU:HD21	1:B:173:VAL:HG22	1.89	0.54
1:B:57:GLY:H	1:B:92:LEU:HD23	1.72	0.54
1:B:465:ILE:HD13	1:B:483:PRO:HG3	1.90	0.54
1:A:185:PHE:HE2	1:A:298:PHE:HB3	0.52	0.53
1:A:26:ARG:CD	1:A:47:LEU:O	2.47	0.53
1:A:392:LEU:HD21	1:A:404:LEU:CD1	2.35	0.53
1:A:128:ARG:HH22	1:A:489:GLN:NE2	1.99	0.53
1:A:226:ILE:HD13	1:A:234:PHE:CD2	2.22	0.53
1:A:234:PHE:HD1	1:A:355:VAL:HB	1.74	0.53
1:A:377:LEU:HD12	1:A:377:LEU:C	2.33	0.53
1:B:426:GLN:OE1	1:B:446:THR:CG2	2.56	0.52
1:B:468:THR:CB	1:B:482:ARG:HD3	2.24	0.52
1:A:418:PRO:HB3	1:B:415:TRP:CZ3	2.43	0.52
1:B:255:GLY:H	1:B:312:ASN:ND2	2.07	0.52
1:B:475:LYS:O	1:B:476:ASP:OD1	2.26	0.52
1:A:128:ARG:NH2	1:A:489:GLN:HE22	2.00	0.52
1:B:468:THR:O	1:B:482:ARG:HD3	2.09	0.52
1:B:250:LEU:HD12	1:B:250:LEU:N	2.24	0.52
1:A:3:LEU:HD21	1:A:173:VAL:HG22	1.92	0.52
1:A:109:VAL:C	1:A:110:LEU:HD12	2.35	0.52
1:A:141:PHE:CE2	1:A:192:LEU:CD2	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:SER:CB	1:B:483:PRO:CG	2.88	0.52
1:B:475:LYS:C	1:B:476:ASP:OD1	2.53	0.52
1:B:193:PRO:O	1:B:193:PRO:CD	2.57	0.51
1:B:377:LEU:HD12	1:B:377:LEU:C	2.35	0.51
1:B:393:MET:SD	1:B:419:LEU:CD2	2.91	0.51
1:A:424:GLN:HE22	1:A:449:CYS:CB	2.23	0.51
1:A:404:LEU:CD1	1:A:404:LEU:N	2.74	0.51
1:B:486:LEU:C	1:B:486:LEU:HD23	2.36	0.51
1:A:234:PHE:CD1	1:A:355:VAL:HB	2.46	0.50
1:B:218:VAL:HG22	1:B:250:LEU:HG	1.91	0.50
1:A:262:PHE:HZ	1:A:369:GLN:NE2	1.95	0.50
1:B:76:VAL:HG21	1:B:92:LEU:CD2	2.42	0.50
1:B:76:VAL:HG21	1:B:92:LEU:HD21	1.89	0.50
1:A:185:PHE:HZ	1:A:298:PHE:CD2	2.29	0.50
1:A:185:PHE:CZ	1:A:298:PHE:CD2	3.00	0.50
1:B:471:ILE:HG23	1:B:473:GLY:O	2.08	0.50
1:A:1:MET:HE1	1:A:134:LEU:CD1	2.39	0.50
1:A:226:ILE:HG23	1:A:234:PHE:CD2	2.46	0.49
1:B:185:PHE:CE2	1:B:298:PHE:CG	3.00	0.49
1:A:475:LYS:O	1:A:476:ASP:OD1	2.29	0.49
1:A:393:MET:HE3	1:A:462:HIS:CD2	2.40	0.49
1:B:1:MET:HE3	1:B:138:GLU:CD	2.37	0.49
1:A:141:PHE:CE2	1:A:192:LEU:HD22	2.47	0.49
1:A:424:GLN:NE2	1:A:449:CYS:CB	2.75	0.49
1:A:3:LEU:CD2	1:A:173:VAL:HG11	2.40	0.49
1:A:185:PHE:CE2	1:A:298:PHE:CB	2.37	0.49
1:B:121:ASP:OD1	1:B:121:ASP:C	2.53	0.49
1:A:26:ARG:CD	1:A:47:LEU:C	2.87	0.48
1:A:373:ASP:OD1	1:A:462:HIS:CA	2.52	0.48
1:A:268:GLY:CA	1:A:291:MET:HG3	2.40	0.48
1:B:185:PHE:CE2	1:B:298:PHE:CB	2.47	0.48
1:B:424:GLN:HE22	1:B:449:CYS:CA	2.24	0.48
1:A:202:LEU:CB	1:A:291:MET:HE1	2.09	0.48
1:B:296:SER:CB	1:B:483:PRO:HG2	2.39	0.48
1:A:426:GLN:OE1	1:A:446:THR:CG2	2.61	0.48
1:B:373:ASP:OD1	1:B:462:HIS:CA	2.53	0.48
1:A:393:MET:HE1	1:A:444:THR:O	2.14	0.47
1:A:404:LEU:CD1	1:A:404:LEU:H	2.28	0.47
1:A:26:ARG:HD3	1:A:47:LEU:C	2.36	0.47
1:A:426:GLN:OE1	1:A:446:THR:HG21	2.14	0.47
1:B:424:GLN:CD	1:B:449:CYS:HB3	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:O	1:A:192:LEU:CD2	2.32	0.47
1:B:223:GLU:HB2	1:B:245:PRO:CD	2.43	0.47
1:A:226:ILE:HD13	1:A:234:PHE:HE2	0.40	0.47
1:A:244:PRO:O	1:A:244:PRO:CD	2.60	0.47
1:A:179:ILE:HG23	1:A:485:PRO:HD3	1.97	0.47
1:B:130:LEU:C	1:B:130:LEU:HD23	2.39	0.47
1:A:330:ARG:O	1:A:331:PRO:C	2.57	0.47
1:B:198:HIS:NE2	1:B:200:SER:HB2	2.29	0.47
1:B:330:ARG:O	1:B:331:PRO:C	2.57	0.46
1:B:76:VAL:HG22	1:B:92:LEU:CD2	2.40	0.46
1:B:26:ARG:HG3	1:B:26:ARG:HH11	1.81	0.46
1:B:244:PRO:O	1:B:244:PRO:CD	2.62	0.46
1:A:132:GLU:OE2	1:A:485:PRO:HG3	2.15	0.45
1:B:1:MET:CE	1:B:154:LEU:HD23	2.46	0.45
1:B:202:LEU:CD2	1:B:291:MET:CE	2.80	0.45
1:B:261:PRO:O	1:B:261:PRO:CD	2.64	0.45
1:A:81:ASP:O	1:A:82:GLU:C	2.60	0.44
1:B:331:PRO:CD	1:B:348:THR:HG23	2.27	0.44
1:A:26:ARG:CD	1:A:47:LEU:HB3	2.47	0.44
1:B:349:ASP:C	1:B:351:GLU:OE1	2.60	0.44
1:A:121:ASP:C	1:A:121:ASP:OD1	2.59	0.44
1:A:484:VAL:HB	1:A:485:PRO:HD2	2.00	0.44
1:A:59:THR:HB	1:A:74:LEU:HD11	2.00	0.43
1:A:486:LEU:HD23	1:A:486:LEU:C	2.43	0.43
1:A:3:LEU:HD22	1:A:173:VAL:CB	2.41	0.43
1:B:393:MET:HE1	1:B:444:THR:O	2.18	0.43
1:B:250:LEU:CD1	1:B:250:LEU:N	2.81	0.43
1:A:392:LEU:O	1:A:416:GLN:HA	2.18	0.43
1:B:7:SER:OG	1:B:163:LYS:HG3	2.18	0.43
1:A:3:LEU:HD22	1:A:173:VAL:HG22	1.93	0.43
1:A:204:GLU:O	1:A:208:GLU:HG3	2.19	0.43
1:B:202:LEU:HD11	1:B:291:MET:SD	2.59	0.43
1:A:221:LEU:HD22	1:A:247:LEU:HD23	2.02	0.42
1:B:121:ASP:OD1	1:B:121:ASP:O	2.38	0.42
1:B:185:PHE:CZ	1:B:298:PHE:CD2	3.07	0.42
1:A:331:PRO:CD	1:A:348:THR:HG23	2.28	0.42
1:A:130:LEU:C	1:A:130:LEU:HD23	2.44	0.42
1:B:181:THR:HG22	1:B:302:ARG:HD3	2.01	0.42
1:A:1:MET:CE	1:A:134:LEU:CD2	2.95	0.41
1:A:268:GLY:O	1:A:319:CYS:HA	2.21	0.41
1:B:226:ILE:CD1	1:B:234:PHE:CZ	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASP:O	1:B:351:GLU:OE1	2.38	0.41
1:B:392:LEU:O	1:B:416:GLN:HA	2.20	0.41
1:B:221:LEU:N	1:B:221:LEU:HD12	2.35	0.41
1:A:97:ALA:O	1:A:101:LYS:HG3	2.20	0.41
1:A:195:ASN:OD1	1:A:195:ASN:C	2.64	0.41
1:A:29:GLY:O	1:A:33:LYS:HG3	2.21	0.41
1:A:442:ALA:HA	1:B:383:VAL:O	2.21	0.40
1:B:234:PHE:HD1	1:B:355:VAL:HB	1.85	0.40
1:B:117:VAL:HG12	1:B:120:ARG:HG3	2.02	0.40
1:B:185:PHE:HZ	1:B:298:PHE:CD2	2.39	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:THR:CB	1:B:214:LYS:CE[4_444]	0.56	1.64
1:B:163:LYS:CE	1:B:164:ALA:O[2_445]	1.27	0.93
1:A:336:THR:CB	1:B:214:LYS:NZ[4_444]	1.56	0.64
1:A:336:THR:OG1	1:B:214:LYS:CE[4_444]	1.60	0.60
1:A:63:GLN:NE2	1:B:49:ARG:NH2[2_455]	1.64	0.56
1:A:336:THR:CG2	1:B:214:LYS:CE[4_444]	1.65	0.55
1:A:336:THR:OG1	1:B:214:LYS:CD[4_444]	1.69	0.51
1:A:336:THR:N	1:B:214:LYS:NZ[4_444]	1.81	0.39
1:A:336:THR:CB	1:B:214:LYS:CD[4_444]	1.89	0.31
1:A:336:THR:CA	1:B:214:LYS:NZ[4_444]	1.94	0.26
1:A:336:THR:OG1	1:B:214:LYS:NZ[4_444]	2.02	0.18
1:A:336:THR:CA	1:B:214:LYS:CE[4_444]	2.03	0.17

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	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
1	B	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
All	All	934/994 (94%)	909 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	359/378 (95%)	358 (100%)	1 (0%)	86	93
1	B	359/378 (95%)	357 (99%)	2 (1%)	78	88
All	All	718/756 (95%)	715 (100%)	3 (0%)	84	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	B	330	ARG
1	B	377	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	A	341	GLN
1	A	424	GLN
1	A	462	HIS
1	A	489	GLN
1	B	63	GLN
1	B	198	HIS
1	B	312	ASN
1	B	424	GLN
1	B	459	ASN

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Mol	Chain	Res	Type
1	B	489	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 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 [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, 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	473/497 (95%)	-1.64	0 100 100	5, 10, 25, 45	0
1	B	473/497 (95%)	-1.61	0 100 100	6, 12, 28, 51	0
All	All	946/994 (95%)	-1.62	0 100 100	5, 11, 27, 51	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 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.