



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:23 AM UTC

PDB ID : 1XAD / pdb_00001xad
Title : CHIMERA ISOPROPYLMALATE DEHYDROGENASE BETWEEN BACILLUS SUBTILIS (M) AND THERMUS THERMOPHILUS (T) FROM N-TERMINAL: 20% T MIDDLE 20% M RESIDUAL 60% T, MUTATED AT S82R. LOW TEMPERATURE (150K) STRUCTURE.
Authors : Nagata, C.; Moriyama, H.; Tanaka, N.
Deposited on : 1995-11-09
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

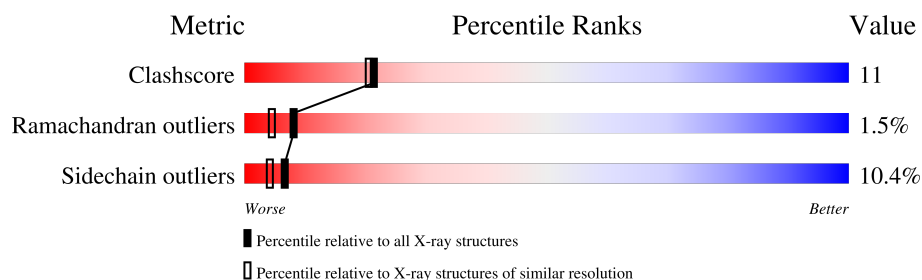
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	 51% 34% 14% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3818 atoms, of which 987 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 2T2M6T S82R.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	H	N	O	S	0	0	0
			3161	1665	549	450	491	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLN	GLY	conflict	UNP P00351
A	80	ASN	LEU	conflict	UNP P00351
A	83	GLU	LYS	conflict	UNP P00351
A	84	LEU	ILE	conflict	UNP P00351
A	85	ARG	SER	conflict	UNP P00351
A	88	LYS	THR	conflict	UNP P00351
A	93	ILE	LEU	conflict	UNP P00351
A	96	GLN	SER	conflict	UNP P00351
A	97	LEU	GLN	conflict	UNP P00351
A	106	VAL	ALA	conflict	UNP P00351
A	110	GLU	PRO	conflict	UNP P00351
A	111	SER	GLY	conflict	UNP P00351
A	113	SER	GLU	conflict	UNP P00351
A	114	ASP	ARG	conflict	UNP P00351
A	115	ALA	LEU	conflict	UNP P00351
A	120	LYS	GLU	conflict	UNP P00351
A	122	TYR	ILE	conflict	UNP P00351
A	123	ILE	ALA	conflict	UNP P00351
A	124	ASP	ARG	conflict	UNP P00351
A	125	ASN	GLY	conflict	UNP P00351
A	128	PHE	VAL	conflict	UNP P00351
A	129	VAL	LEU	conflict	UNP P00351

- Molecule 2 is water.

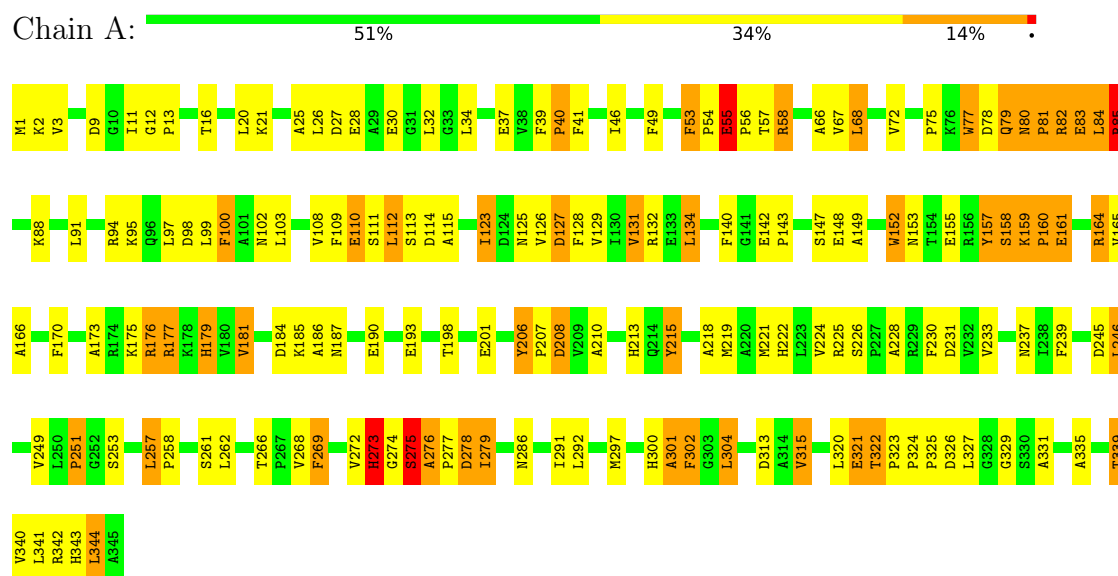
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	219	Total	H	O	0	0
			657	438	219		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE 2T2M6T S82R



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.40 Å 77.40 Å 156.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3818	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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	1.42	21/2668 (0.8%)	2.24	135/3621 (3.7%)

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

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	HIS	CG-ND1	-8.47	1.28	1.38
1	A	131	VAL	CA-CB	7.70	1.63	1.54
1	A	222	HIS	CD2-NE2	-7.34	1.29	1.37
1	A	213	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	273	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	161	GLU	CA-CB	-6.24	1.43	1.53
1	A	40	PRO	CA-CB	-6.20	1.45	1.53
1	A	179	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	275	SER	CA-CB	-6.01	1.44	1.53
1	A	326	ASP	CA-CB	5.99	1.63	1.53
1	A	273	HIS	ND1-CE1	-5.84	1.26	1.32
1	A	343	HIS	CG-ND1	-5.74	1.31	1.38
1	A	300	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	134	LEU	CA-CB	-5.67	1.46	1.54
1	A	222	HIS	CG-ND1	-5.58	1.32	1.38
1	A	273	HIS	CG-ND1	-5.57	1.32	1.38
1	A	9	ASP	CA-CB	-5.46	1.45	1.53
1	A	54	PRO	CA-CB	-5.44	1.47	1.53
1	A	343	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	315	VAL	CA-CB	5.21	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ARG	NE-CZ	5.02	1.38	1.33

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ASP	CA-CB-CG	13.06	125.66	112.60
1	A	179	HIS	CB-CG-CD2	-11.07	116.81	131.20
1	A	273	HIS	CA-CB-CG	10.85	124.65	113.80
1	A	321	GLU	N-CA-C	10.79	123.13	111.36
1	A	278	ASP	CA-CB-CG	10.65	123.25	112.60
1	A	46	ILE	N-CA-C	-10.12	101.02	110.53
1	A	273	HIS	CB-CG-CD2	-9.96	118.25	131.20
1	A	102	ASN	OD1-CG-ND2	-8.77	113.83	122.60
1	A	326	ASP	CA-CB-CG	8.55	121.15	112.60
1	A	286	ASN	OD1-CG-ND2	-8.50	114.10	122.60
1	A	127	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	77	TRP	CG-CD2-CE3	8.09	141.99	133.90
1	A	224	VAL	N-CA-C	-8.03	105.39	111.90
1	A	164	ARG	CB-CG-CD	-7.80	93.36	111.30
1	A	140	PHE	CA-C-N	7.73	127.45	120.10
1	A	140	PHE	C-N-CA	7.73	127.45	120.10
1	A	226	SER	O-C-N	-7.54	114.86	121.20
1	A	237	ASN	N-CA-C	7.39	119.23	111.03
1	A	128	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	67	VAL	CA-C-O	-7.16	112.55	120.72
1	A	159	LYS	CA-C-N	7.16	126.68	119.24
1	A	159	LYS	C-N-CA	7.16	126.68	119.24
1	A	273	HIS	CG-CD2-NE2	-7.14	100.06	107.20
1	A	315	VAL	N-CA-CB	7.11	121.25	110.58
1	A	84	LEU	N-CA-C	-7.08	102.22	111.71
1	A	179	HIS	CB-CA-C	-6.97	97.46	109.65
1	A	16	THR	N-CA-CB	6.95	120.44	110.16
1	A	179	HIS	CB-CG-ND1	6.91	133.06	122.70
1	A	26	LEU	N-CA-C	-6.89	103.70	111.14
1	A	315	VAL	CB-CA-C	-6.85	102.76	112.22
1	A	161	GLU	CB-CG-CD	-6.80	101.05	112.60
1	A	274	GLY	CA-C-N	6.79	129.38	120.28
1	A	274	GLY	C-N-CA	6.79	129.38	120.28
1	A	56	PRO	CA-N-CD	-6.77	102.52	112.00
1	A	187	ASN	OD1-CG-ND2	-6.77	115.83	122.60
1	A	129	VAL	CA-C-O	-6.72	113.48	120.27
1	A	179	HIS	N-CA-CB	6.72	122.10	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	LEU	N-CA-C	6.71	120.45	110.32
1	A	16	THR	CB-CA-C	-6.69	99.48	110.85
1	A	315	VAL	CA-C-O	-6.58	113.87	120.85
1	A	55	GLU	CA-C-O	-6.56	111.62	117.98
1	A	269	PHE	CA-CB-CG	-6.51	107.29	113.80
1	A	268	VAL	O-C-N	-6.47	116.07	122.93
1	A	273	HIS	CE1-NE2-CD2	6.45	115.45	109.00
1	A	313	ASP	CB-CA-C	-6.43	100.74	110.90
1	A	176	ARG	O-C-N	-6.42	114.05	122.59
1	A	177	ARG	N-CA-C	6.40	124.43	110.80
1	A	210	ALA	CA-C-O	-6.38	113.59	120.92
1	A	41	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	125	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	186	ALA	N-CA-C	6.24	120.16	112.54
1	A	149	ALA	N-CA-C	6.21	119.33	111.69
1	A	58	ARG	CA-CB-CG	6.20	126.49	114.10
1	A	181	VAL	O-C-N	-6.15	116.68	123.20
1	A	340	VAL	CB-CA-C	-6.14	104.11	111.97
1	A	100	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	153	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	3	VAL	CA-C-O	-6.05	113.58	120.66
1	A	20	LEU	CA-C-O	-6.04	114.43	120.90
1	A	82	ARG	N-CA-C	-6.01	98.01	110.80
1	A	181	VAL	CA-C-O	-6.00	114.15	120.39
1	A	201	GLU	CA-CB-CG	-6.00	102.10	114.10
1	A	327	LEU	N-CA-C	-6.00	103.68	111.71
1	A	185	LYS	N-CA-C	-5.99	103.26	110.44
1	A	27	ASP	CA-C-O	-5.93	114.55	120.90
1	A	53	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	322	THR	O-C-N	-5.87	116.18	121.17
1	A	77	TRP	CB-CG-CD1	-5.86	118.12	126.90
1	A	302	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	91	LEU	N-CA-C	-5.78	106.36	113.41
1	A	193	GLU	CA-C-N	5.76	128.26	120.65
1	A	193	GLU	C-N-CA	5.76	128.26	120.65
1	A	213	HIS	CA-C-O	-5.72	114.74	121.44
1	A	112	LEU	N-CA-C	-5.72	106.19	112.72
1	A	85	ARG	CA-C-N	5.71	125.39	119.05
1	A	85	ARG	C-N-CA	5.71	125.39	119.05
1	A	276	ALA	O-C-N	-5.70	114.77	121.32
1	A	147	SER	CA-C-O	-5.67	114.91	121.49
1	A	26	LEU	CA-C-O	-5.66	114.87	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLU	N-CA-C	-5.66	100.07	109.46
1	A	152	TRP	CG-CD2-CE3	5.64	139.54	133.90
1	A	55	GLU	CA-C-N	5.62	125.09	119.24
1	A	55	GLU	C-N-CA	5.62	125.09	119.24
1	A	37	GLU	O-C-N	-5.60	116.53	123.36
1	A	245	ASP	O-C-N	-5.59	116.31	122.07
1	A	57	THR	CA-C-O	-5.58	114.50	120.42
1	A	274	GLY	O-C-N	5.55	129.51	122.85
1	A	320	LEU	CA-C-O	-5.55	114.98	120.70
1	A	67	VAL	O-C-N	-5.55	117.48	123.14
1	A	2	LYS	CG-CD-CE	-5.55	98.54	111.30
1	A	222	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	206	TYR	CA-C-N	5.52	126.74	119.84
1	A	206	TYR	C-N-CA	5.52	126.74	119.84
1	A	208	ASP	N-CA-C	5.51	119.87	113.20
1	A	79	GLN	CA-C-O	-5.50	115.05	120.82
1	A	279	ILE	N-CA-C	5.49	117.48	112.43
1	A	233	VAL	O-C-N	-5.45	117.37	123.26
1	A	166	ALA	O-C-N	-5.42	115.97	122.15
1	A	225	ARG	N-CA-C	5.42	118.36	111.69
1	A	291	ILE	O-C-N	-5.41	116.59	121.89
1	A	148	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	340	VAL	N-CA-C	-5.39	105.24	110.42
1	A	39	PHE	CA-C-O	-5.39	115.11	120.66
1	A	21	LYS	CA-C-O	-5.38	115.15	120.90
1	A	68	LEU	N-CA-C	-5.38	98.48	107.99
1	A	12	GLY	CA-C-N	5.36	124.81	119.24
1	A	12	GLY	C-N-CA	5.36	124.81	119.24
1	A	343	HIS	CA-C-N	-5.33	114.10	122.79
1	A	343	HIS	C-N-CA	-5.33	114.10	122.79
1	A	25	ALA	CB-CA-C	-5.33	101.94	110.79
1	A	215	TYR	O-C-N	-5.31	117.11	123.06
1	A	343	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	268	VAL	CA-C-O	-5.30	114.69	120.84
1	A	158	SER	N-CA-CB	-5.29	102.70	110.85
1	A	226	SER	N-CA-CB	-5.29	103.34	110.74
1	A	273	HIS	CB-CG-ND1	5.20	130.50	122.70
1	A	198	THR	CA-C-O	-5.20	115.36	120.82
1	A	85	ARG	O-C-N	-5.17	117.36	121.80
1	A	58	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	123	ILE	CB-CA-C	-5.15	104.39	111.65
1	A	320	LEU	N-CA-C	-5.15	105.58	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	PRO	CA-N-CD	-5.14	104.81	112.00
1	A	273	HIS	ND1-CG-CD2	5.13	111.23	106.10
1	A	340	VAL	N-CA-CB	5.12	116.55	110.55
1	A	98	ASP	N-CA-C	5.12	118.39	111.17
1	A	72	VAL	N-CA-C	5.10	116.53	109.29
1	A	66	ALA	CA-C-O	-5.08	115.30	120.89
1	A	276	ALA	CA-C-O	5.08	123.98	120.47
1	A	125	ASN	CB-CG-ND2	5.07	124.00	116.40
1	A	239	PHE	CA-C-O	-5.06	114.15	119.97
1	A	301	ALA	N-CA-C	-5.06	104.75	112.04
1	A	155	GLU	CA-C-O	-5.04	114.85	120.54
1	A	57	THR	CA-CB-OG1	-5.03	102.05	109.60
1	A	213	HIS	CA-CB-CG	-5.01	108.79	113.80
1	A	77	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	Sidechain
1	A	80	ASN	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	2612	549	2630	57	0
2	A	219	438	0	4	1
All	All	2831	987	2630	57	1

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 11.

All (57) 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:94:ARG:HD2	1:A:134:LEU:HD13	1.58	0.85
1:A:30:GLU:HB2	1:A:32:LEU:HD12	1.64	0.80
1:A:325:PRO:HA	1:A:329:GLY:O	1.90	0.72
1:A:83:GLU:HA	1:A:88:LYS:HG3	1.75	0.68
1:A:112:LEU:HB2	2:A:583:HOH:O	1.96	0.66
1:A:103:LEU:HD13	1:A:262:LEU:HD22	1.78	0.65
1:A:246:LEU:O	1:A:249:VAL:HG22	1.99	0.61
1:A:97:LEU:HD23	1:A:266:THR:O	2.03	0.57
1:A:159:LYS:N	1:A:160:PRO:HD2	2.20	0.56
1:A:181:VAL:HG21	1:A:230:PHE:HD1	1.71	0.56
1:A:108:VAL:HG22	1:A:251:PRO:HA	1.89	0.54
1:A:292:LEU:HD21	1:A:315:VAL:HG21	1.89	0.54
1:A:218:ALA:HA	1:A:221:MET:HE3	1.88	0.54
1:A:302:PHE:O	1:A:304:LEU:HD13	2.09	0.53
1:A:339:THR:HA	1:A:342:ARG:HB3	1.91	0.53
1:A:335:ALA:O	1:A:339:THR:HG22	2.09	0.53
1:A:30:GLU:HB2	1:A:32:LEU:CD1	2.38	0.52
1:A:341:LEU:HA	1:A:344:LEU:CD2	2.41	0.51
1:A:40:PRO:HG3	1:A:49:PHE:CE2	2.46	0.50
1:A:170:PHE:O	1:A:173:ALA:HB3	2.11	0.50
1:A:81:PRO:HD2	1:A:84:LEU:HB2	1.94	0.50
1:A:323:PRO:HG2	1:A:329:GLY:HA3	1.93	0.50
1:A:99:LEU:HD13	1:A:261:SER:HB2	1.93	0.49
1:A:1:MET:HG3	1:A:302:PHE:CE2	2.48	0.49
1:A:11:ILE:HG12	1:A:275:SER:O	2.13	0.49
1:A:325:PRO:HD3	1:A:331:ALA:O	2.14	0.47
1:A:100:PHE:CE1	1:A:164:ARG:HB3	2.50	0.47
1:A:272:VAL:O	1:A:273:HIS:HB3	2.15	0.47
1:A:77:TRP:HA	1:A:80:ASN:OD1	2.15	0.47
1:A:322:THR:OG1	1:A:339:THR:HG21	2.14	0.47
1:A:127:ASP:HB3	1:A:177:ARG:HH12	1.80	0.47
1:A:276:ALA:N	1:A:277:PRO:HD3	2.30	0.46
1:A:123:ILE:O	1:A:126:VAL:HG23	2.15	0.46
1:A:160:PRO:HG2	1:A:161:GLU:H	1.80	0.46
1:A:184:ASP:O	1:A:215:TYR:HA	2.17	0.45
1:A:1:MET:N	2:A:727:HOH:O	2.49	0.45
1:A:341:LEU:HA	1:A:344:LEU:HD22	1.98	0.45
1:A:75:PRO:HA	1:A:78:ASP:OD2	2.17	0.44
1:A:78:ASP:HA	1:A:85:ARG:HD2	1.99	0.44
1:A:297:MET:O	1:A:301:ALA:HB3	2.18	0.44
1:A:269:PHE:CZ	1:A:297:MET:HA	2.54	0.43
1:A:181:VAL:HG21	1:A:230:PHE:CD1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:HA	1:A:58:ARG:HB2	2.00	0.43
1:A:158:SER:C	1:A:160:PRO:HD2	2.44	0.43
1:A:257:LEU:HA	1:A:258:PRO:HD3	1.94	0.42
1:A:278:ASP:OD2	1:A:279:ILE:HG23	2.19	0.42
1:A:99:LEU:HD13	1:A:261:SER:CB	2.49	0.42
1:A:219:MET:HE1	1:A:230:PHE:CE2	2.54	0.42
1:A:177:ARG:NH2	1:A:231:ASP:HA	2.34	0.42
1:A:113:SER:O	1:A:115:ALA:N	2.53	0.42
1:A:109:PHE:O	1:A:110:GLU:C	2.63	0.42
1:A:206:TYR:O	1:A:208:ASP:N	2.52	0.41
1:A:179:HIS:O	1:A:231:ASP:HB3	2.20	0.41
1:A:132:ARG:HD3	2:A:614:HOH:O	2.20	0.41
1:A:109:PHE:HB3	2:A:642:HOH:O	2.20	0.40
1:A:142:GLU:CG	1:A:143:PRO:HA	2.52	0.40
1:A:53:PHE:CD2	1:A:58:ARG:HD2	2.56	0.40

All (1) 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)
2:A:485:HOH:H1	2:A:485:HOH:H1[4_556]	1.21	0.39

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%)	26 (8%)	5 (2%)	8 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	HIS
1	A	228	ALA
1	A	28	GLU
1	A	207	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	270/270 (100%)	242 (90%)	28 (10%)	7 4

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	34	LEU
1	A	55	GLU
1	A	68	LEU
1	A	79	GLN
1	A	82	ARG
1	A	83	GLU
1	A	85	ARG
1	A	95	LYS
1	A	110	GLU
1	A	111	SER
1	A	131	VAL
1	A	152	TRP
1	A	157	TYR
1	A	165	VAL
1	A	175	LYS
1	A	176	ARG
1	A	190	GLU
1	A	246	LEU
1	A	251	PRO
1	A	253	SER
1	A	273	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	275	SER
1	A	304	LEU
1	A	321	GLU
1	A	324	PRO
1	A	339	THR
1	A	344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	102	ASN
1	A	222	HIS
1	A	300	HIS

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.