



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:20 PM UTC

PDB ID : 1BSF / pdb_00001bsf
Title : THERMOSTABLE THYMIDYLATE SYNTHASE A FROM BACILLUS SUBTILIS
Authors : Stout, T.J.; Schellenberger, U.; Santi, D.V.; Stroud, R.M.
Deposited on : 1998-07-10
Resolution : 2.20 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

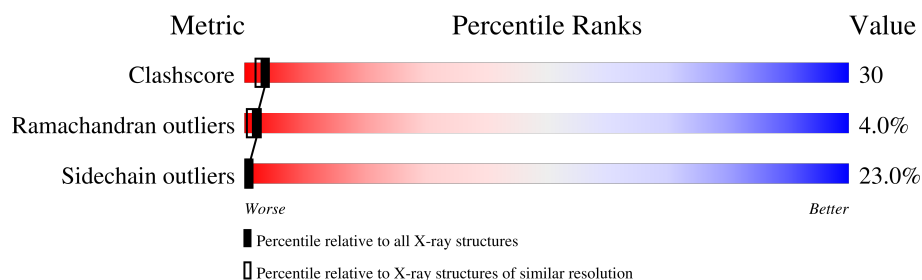
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

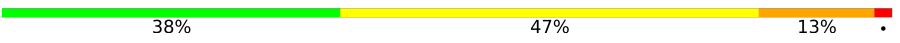
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	278	 38% 47% 13% •
1	B	278	 37% 48% 13% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4602 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 THYMIDYLATE SYNTHASE A.

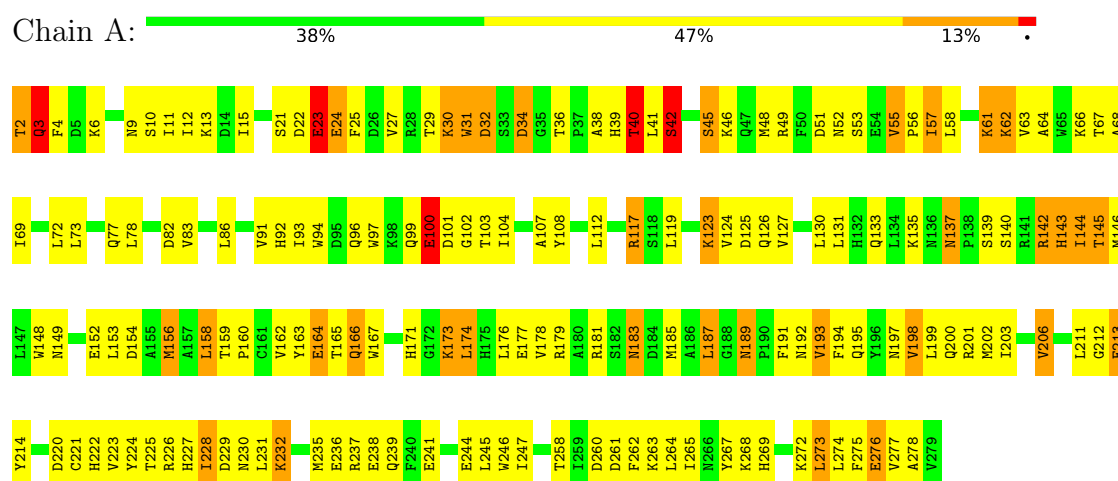
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2301	1471	390	430	10			
1	B	278	Total	C	N	O	S	0	0	0
			2301	1471	390	430	10			

3 Residue-property plots

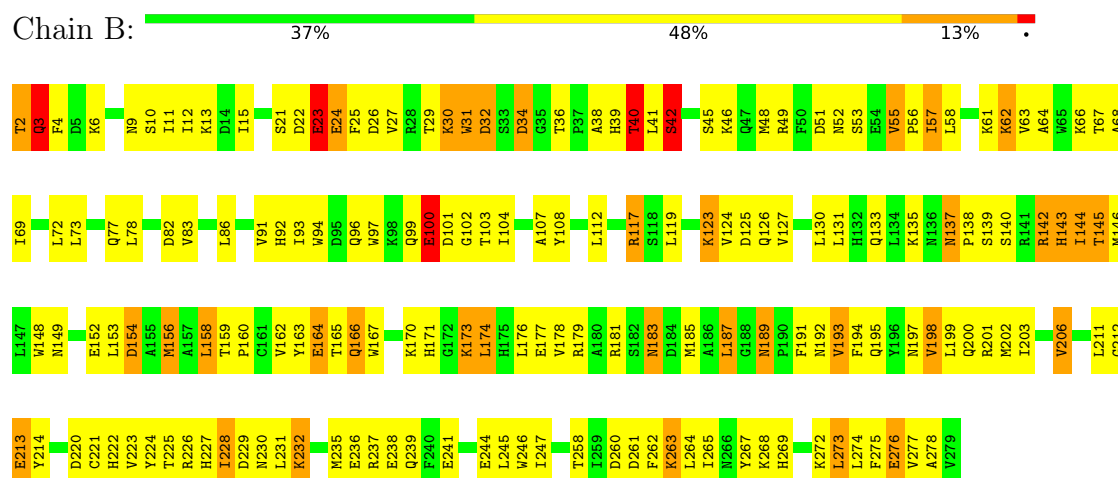
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: THYMIDYLATE SYNTHASE A



• Molecule 1: THYMIDYLATE SYNTHASE A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.98Å 95.96Å 143.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.20	Depositor
% Data completeness (in resolution range)	23.1 (60.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.854	Depositor
R, R_{free}	0.195 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4602	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	0.42	0/2359	0.92	8/3196 (0.3%)
1	B	0.42	0/2359	0.92	8/3196 (0.3%)
All	All	0.42	0/4718	0.92	16/6392 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	VAL	N-CA-C	-6.50	104.31	110.42
1	A	198	VAL	N-CA-C	-6.49	104.32	110.42
1	B	189	ASN	N-CA-C	6.45	121.25	112.55
1	A	189	ASN	N-CA-C	6.42	121.22	112.55
1	B	53	SER	N-CA-C	-6.28	105.62	113.28
1	A	53	SER	N-CA-C	-6.26	105.64	113.28
1	A	265	ILE	N-CA-C	5.93	116.84	108.36
1	B	265	ILE	N-CA-C	5.89	116.79	108.36
1	A	144	ILE	N-CA-C	5.63	116.38	108.17
1	B	144	ILE	N-CA-C	5.61	116.36	108.17
1	B	42	SER	N-CA-C	5.28	116.82	108.96
1	B	40	THR	N-CA-C	5.27	117.28	109.69
1	A	42	SER	N-CA-C	5.26	116.80	108.96
1	A	40	THR	N-CA-C	5.25	117.26	109.69
1	A	228	ILE	N-CA-C	5.15	115.30	110.30
1	B	228	ILE	N-CA-C	5.14	115.29	110.30

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	2301	0	2226	136	6
1	B	2301	0	2226	140	6
All	All	4602	0	4452	269	8

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 30.

All (269) 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:12:ILE:HD12	1:B:231:LEU:HD13	1.40	1.01
1:A:12:ILE:HD12	1:A:231:LEU:HD13	1.41	1.00
1:B:107:ALA:HB2	1:B:156:MET:HB3	1.44	0.99
1:A:229:ASP:HA	1:A:232:LYS:HD2	1.41	0.98
1:B:229:ASP:HA	1:B:232:LYS:HD2	1.41	0.98
1:A:107:ALA:HB2	1:A:156:MET:HB3	1.44	0.97
1:A:167:TRP:HE3	1:A:174:LEU:HD11	1.31	0.94
1:B:167:TRP:HE3	1:B:174:LEU:HD11	1.31	0.94
1:A:176:LEU:HD23	1:A:200:GLN:HB2	1.50	0.91
1:B:176:LEU:HD23	1:B:200:GLN:HB2	1.50	0.90
1:A:127:VAL:O	1:A:131:LEU:HG	1.76	0.86
1:B:127:VAL:O	1:B:131:LEU:HG	1.76	0.86
1:B:42:SER:HB3	1:B:222:HIS:HB3	1.62	0.82
1:A:42:SER:HB3	1:A:222:HIS:HB3	1.62	0.81
1:B:228:ILE:HG22	1:B:232:LYS:HE2	1.67	0.77
1:A:228:ILE:HG22	1:A:232:LYS:HE2	1.67	0.76
1:A:3:GLN:HE21	1:A:4:PHE:N	1.86	0.73
1:A:49:ARG:HB3	1:A:213:GLU:OE2	1.90	0.72
1:B:3:GLN:HE21	1:B:4:PHE:N	1.86	0.72
1:B:49:ARG:HB3	1:B:213:GLU:OE2	1.90	0.71
1:B:34:ASP:HB2	1:B:36:THR:HG23	1.74	0.70
1:A:34:ASP:HB2	1:A:36:THR:HG23	1.74	0.69
1:B:202:MET:O	1:B:206:VAL:HG13	1.92	0.69
1:A:202:MET:O	1:A:206:VAL:HG13	1.92	0.69
1:A:229:ASP:CA	1:A:232:LYS:HD2	2.20	0.69
1:A:3:GLN:NE2	1:A:4:PHE:H	1.90	0.69
1:B:229:ASP:CA	1:B:232:LYS:HD2	2.20	0.69
1:B:3:GLN:NE2	1:B:4:PHE:H	1.90	0.69
1:A:230:ASN:HB3	1:A:275:PHE:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:O	1:A:25:PHE:N	2.26	0.68
1:B:23:GLU:O	1:B:25:PHE:N	2.27	0.67
1:A:31:TRP:CE3	1:A:278:ALA:HB2	2.30	0.67
1:B:230:ASN:HB3	1:B:275:PHE:CE1	2.29	0.67
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.59	0.67
1:B:100:GLU:H	1:B:100:GLU:CD	2.02	0.67
1:B:149:ASN:ND2	1:B:152:GLU:HG3	2.10	0.67
1:B:31:TRP:CE3	1:B:278:ALA:HB2	2.30	0.67
1:B:57:ILE:HD11	1:B:63:VAL:HB	1.77	0.67
1:A:25:PHE:CE1	1:B:138:PRO:HG2	2.30	0.67
1:A:173:LYS:HG2	1:A:212:GLY:HA2	1.76	0.67
1:A:149:ASN:ND2	1:A:152:GLU:HG3	2.10	0.66
1:B:32:ASP:HB2	1:B:277:VAL:HG23	1.78	0.66
1:B:173:LYS:HG2	1:B:212:GLY:HA2	1.76	0.66
1:B:167:TRP:CE3	1:B:174:LEU:HD11	2.23	0.66
1:A:32:ASP:HB2	1:A:277:VAL:HG23	1.78	0.66
1:B:179:ARG:HG2	1:B:179:ARG:HH11	1.59	0.65
1:B:231:LEU:O	1:B:235:MET:HG2	1.97	0.65
1:A:231:LEU:O	1:A:235:MET:HG2	1.97	0.65
1:A:57:ILE:HD11	1:A:63:VAL:HB	1.77	0.65
1:A:100:GLU:CD	1:A:100:GLU:H	2.02	0.64
1:A:62:LYS:HG3	1:A:269:HIS:NE2	2.12	0.64
1:B:62:LYS:HG3	1:B:269:HIS:NE2	2.12	0.63
1:B:183:ASN:HD21	1:B:192:ASN:HD22	1.47	0.62
1:B:55:VAL:HG12	1:B:57:ILE:HG22	1.82	0.62
1:B:130:LEU:HD22	1:B:145:THR:HG22	1.81	0.62
1:A:130:LEU:HD22	1:A:145:THR:HG22	1.81	0.61
1:A:55:VAL:HG12	1:A:57:ILE:HG22	1.82	0.61
1:A:183:ASN:HD21	1:A:192:ASN:HD22	1.47	0.61
1:A:183:ASN:HD21	1:A:192:ASN:ND2	1.99	0.61
1:A:153:LEU:HD13	1:B:117:ARG:NH1	2.17	0.60
1:B:4:PHE:HE2	1:B:58:LEU:HG	1.66	0.60
1:A:167:TRP:CH2	1:A:176:LEU:HD22	2.37	0.60
1:B:167:TRP:CH2	1:B:176:LEU:HD22	2.37	0.60
1:B:11:ILE:O	1:B:15:ILE:HG13	2.02	0.59
1:A:167:TRP:CE3	1:A:174:LEU:HD11	2.23	0.59
1:B:3:GLN:NE2	1:B:4:PHE:N	2.49	0.59
1:A:4:PHE:HE2	1:A:58:LEU:HG	1.66	0.59
1:B:4:PHE:CE2	1:B:58:LEU:HG	2.37	0.59
1:A:4:PHE:CE2	1:A:58:LEU:HG	2.37	0.59
1:A:69:ILE:HG12	1:A:198:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:NE2	1:A:4:PHE:N	2.49	0.59
1:A:11:ILE:O	1:A:15:ILE:HG13	2.02	0.59
1:B:183:ASN:HD21	1:B:192:ASN:ND2	1.99	0.59
1:B:40:THR:HB	1:B:223:VAL:O	2.03	0.58
1:A:247:ILE:HG12	1:A:262:PHE:CD1	2.38	0.58
1:A:264:LEU:HD23	1:A:267:TYR:CD2	2.38	0.58
1:B:144:ILE:HG12	1:B:166:GLN:HG2	1.85	0.58
1:B:264:LEU:HD23	1:B:267:TYR:CD2	2.38	0.58
1:B:247:ILE:HG12	1:B:262:PHE:CD1	2.38	0.58
1:A:112:LEU:HD22	1:A:127:VAL:HG23	1.85	0.57
1:A:144:ILE:HG12	1:A:166:GLN:HG2	1.85	0.57
1:A:40:THR:HB	1:A:223:VAL:O	2.03	0.57
1:A:173:LYS:HG2	1:A:212:GLY:CA	2.35	0.57
1:B:112:LEU:HD22	1:B:127:VAL:HG23	1.84	0.57
1:B:69:ILE:HG12	1:B:198:VAL:HG11	1.85	0.57
1:A:48:MET:HE1	1:A:193:VAL:HG21	1.86	0.56
1:A:68:ALA:HA	1:A:191:PHE:CZ	2.41	0.56
1:A:82:ASP:HA	1:A:103:THR:HG22	1.87	0.56
1:A:228:ILE:CG2	1:A:232:LYS:HE2	2.35	0.56
1:B:48:MET:HE1	1:B:193:VAL:HG21	1.86	0.56
1:B:68:ALA:HA	1:B:191:PHE:CZ	2.41	0.56
1:B:173:LYS:HG2	1:B:212:GLY:CA	2.35	0.56
1:B:82:ASP:HA	1:B:103:THR:HG22	1.87	0.56
1:B:56:PRO:O	1:B:194:PHE:HB2	2.05	0.56
1:B:31:TRP:CE2	1:B:226:ARG:HG3	2.41	0.55
1:A:56:PRO:O	1:A:194:PHE:HB2	2.05	0.55
1:A:108:TYR:OH	1:A:160:PRO:HA	2.06	0.55
1:A:237:ARG:HG3	1:A:238:GLU:H	1.72	0.55
1:A:237:ARG:HG3	1:A:238:GLU:N	2.21	0.55
1:A:22:ASP:CG	1:A:39:HIS:HD1	2.15	0.55
1:B:108:TYR:OH	1:B:160:PRO:HA	2.06	0.55
1:B:228:ILE:CG2	1:B:232:LYS:HE2	2.35	0.55
1:A:31:TRP:CE2	1:A:226:ARG:HG3	2.41	0.55
1:B:22:ASP:CG	1:B:39:HIS:HD1	2.15	0.55
1:B:237:ARG:HG3	1:B:238:GLU:H	1.72	0.55
1:B:34:ASP:C	1:B:36:THR:H	2.15	0.54
1:A:34:ASP:C	1:A:36:THR:H	2.15	0.54
1:B:23:GLU:C	1:B:25:PHE:H	2.16	0.54
1:B:237:ARG:HG3	1:B:238:GLU:N	2.21	0.54
1:A:31:TRP:CZ2	1:A:226:ARG:HB2	2.43	0.54
1:B:229:ASP:HA	1:B:232:LYS:CD	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:C	1:A:25:PHE:H	2.16	0.54
1:A:112:LEU:HD22	1:A:127:VAL:CG2	2.37	0.54
1:B:31:TRP:CZ2	1:B:226:ARG:HB2	2.43	0.54
1:A:83:VAL:HG23	1:A:102:GLY:O	2.08	0.54
1:B:108:TYR:HE2	1:B:158:LEU:HD13	1.74	0.53
1:B:112:LEU:HD22	1:B:127:VAL:CG2	2.37	0.53
1:B:83:VAL:HG23	1:B:102:GLY:O	2.08	0.53
1:A:229:ASP:HA	1:A:232:LYS:CD	2.26	0.52
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.24	0.52
1:B:179:ARG:HG2	1:B:179:ARG:NH1	2.24	0.52
1:A:92:HIS:C	1:A:94:TRP:H	2.18	0.52
1:A:9:ASN:ND2	1:A:235:MET:HA	2.25	0.52
1:A:108:TYR:HE2	1:A:158:LEU:HD13	1.74	0.52
1:B:272:LYS:O	1:B:273:LEU:HD23	2.10	0.52
1:B:9:ASN:ND2	1:B:235:MET:HA	2.25	0.51
1:A:272:LYS:O	1:A:273:LEU:HD23	2.10	0.51
1:B:174:LEU:C	1:B:174:LEU:HD12	2.35	0.51
1:A:23:GLU:C	1:A:25:PHE:N	2.69	0.51
1:B:92:HIS:C	1:B:94:TRP:H	2.18	0.51
1:A:276:GLU:CD	1:A:276:GLU:H	2.19	0.50
1:B:276:GLU:H	1:B:276:GLU:CD	2.19	0.50
1:A:174:LEU:C	1:A:174:LEU:HD12	2.35	0.50
1:A:176:LEU:HD12	1:A:177:GLU:N	2.27	0.50
1:B:6:LYS:NZ	1:B:239:GLN:OE1	2.45	0.50
1:B:176:LEU:HD12	1:B:177:GLU:N	2.27	0.49
1:B:23:GLU:C	1:B:25:PHE:N	2.69	0.49
1:B:2:THR:O	1:B:3:GLN:C	2.56	0.49
1:A:30:LYS:HA	1:A:38:ALA:H	1.77	0.49
1:A:2:THR:O	1:A:3:GLN:C	2.56	0.48
1:A:142:ARG:O	1:A:144:ILE:N	2.46	0.48
1:B:142:ARG:O	1:B:144:ILE:N	2.46	0.48
1:A:6:LYS:NZ	1:A:239:GLN:OE1	2.45	0.48
1:A:22:ASP:OD2	1:A:27:VAL:HG11	2.14	0.48
1:A:63:VAL:HG12	1:A:64:ALA:N	2.27	0.48
1:B:63:VAL:HG12	1:B:64:ALA:N	2.27	0.48
1:B:86:LEU:HG	1:B:91:VAL:HB	1.96	0.48
1:B:22:ASP:OD2	1:B:27:VAL:HG11	2.14	0.48
1:B:30:LYS:HA	1:B:38:ALA:H	1.77	0.48
1:B:174:LEU:O	1:B:212:GLY:N	2.43	0.47
1:B:189:ASN:O	1:B:193:VAL:HG23	2.14	0.47
1:A:189:ASN:O	1:A:193:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:HG2	1:A:201:ARG:HH11	1.79	0.47
1:A:245:LEU:HD12	1:A:246:TRP:N	2.29	0.47
1:A:112:LEU:O	1:A:125:ASP:HB2	2.15	0.47
1:B:176:LEU:CD2	1:B:200:GLN:HB2	2.34	0.47
1:A:86:LEU:HG	1:A:91:VAL:HB	1.96	0.47
1:B:112:LEU:O	1:B:125:ASP:HB2	2.15	0.47
1:B:245:LEU:HD12	1:B:246:TRP:N	2.29	0.47
1:A:11:ILE:HG21	1:A:185:MET:HE2	1.97	0.46
1:B:201:ARG:HH11	1:B:201:ARG:HG2	1.79	0.46
1:B:230:ASN:OD1	1:B:273:LEU:HD13	2.15	0.46
1:A:72:LEU:HD11	1:A:199:LEU:HB2	1.97	0.46
1:A:117:ARG:NH2	1:B:154:ASP:OD1	2.47	0.46
1:A:230:ASN:OD1	1:A:273:LEU:HD13	2.15	0.46
1:A:92:HIS:O	1:A:94:TRP:N	2.49	0.46
1:A:133:GLN:OE1	1:A:133:GLN:HA	2.15	0.46
1:B:72:LEU:HD11	1:B:199:LEU:HB2	1.97	0.46
1:A:140:SER:HB3	1:A:143:HIS:CE1	2.51	0.46
1:A:224:TYR:CD1	1:A:224:TYR:N	2.83	0.46
1:B:31:TRP:CZ2	1:B:226:ARG:HG3	2.51	0.46
1:A:64:ALA:HB3	1:A:191:PHE:CD1	2.51	0.46
1:A:117:ARG:NH1	1:B:153:LEU:HD13	2.31	0.46
1:B:11:ILE:HG21	1:B:185:MET:HE2	1.97	0.46
1:B:133:GLN:HA	1:B:133:GLN:OE1	2.15	0.46
1:B:140:SER:HB3	1:B:143:HIS:CE1	2.51	0.46
1:B:224:TYR:N	1:B:224:TYR:CD1	2.83	0.46
1:A:145:THR:HG23	1:A:165:THR:OG1	2.16	0.46
1:B:163:TYR:OH	1:B:179:ARG:NH1	2.49	0.46
1:A:163:TYR:OH	1:A:179:ARG:NH1	2.49	0.46
1:A:41:LEU:CD1	1:A:228:ILE:HD11	2.46	0.45
1:A:63:VAL:CG1	1:A:64:ALA:N	2.79	0.45
1:A:176:LEU:CD2	1:A:200:GLN:HB2	2.34	0.45
1:B:41:LEU:CD1	1:B:228:ILE:HD11	2.46	0.45
1:B:57:ILE:HG13	1:B:58:LEU:N	2.32	0.45
1:B:145:THR:HG23	1:B:165:THR:OG1	2.16	0.45
1:A:57:ILE:HG13	1:A:58:LEU:N	2.32	0.45
1:A:167:TRP:CZ3	1:A:176:LEU:HD22	2.51	0.45
1:B:63:VAL:CG1	1:B:64:ALA:N	2.79	0.45
1:B:92:HIS:O	1:B:94:TRP:N	2.49	0.45
1:A:55:VAL:HG12	1:A:57:ILE:CG2	2.46	0.45
1:A:247:ILE:HA	1:A:261:ASP:O	2.16	0.45
1:A:31:TRP:CZ2	1:A:226:ARG:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:O	1:B:143:HIS:HE1	2.00	0.45
1:B:64:ALA:HB3	1:B:191:PHE:CD1	2.51	0.45
1:B:167:TRP:CZ3	1:B:176:LEU:HD22	2.51	0.45
1:B:117:ARG:O	1:B:123:LYS:HA	2.17	0.45
1:B:126:GLN:OE1	1:B:145:THR:HA	2.17	0.45
1:B:191:PHE:O	1:B:195:GLN:HB3	2.17	0.45
1:A:31:TRP:HE3	1:A:278:ALA:HB2	1.81	0.45
1:A:191:PHE:O	1:A:195:GLN:HB3	2.17	0.45
1:A:163:TYR:HD1	1:A:163:TYR:H	1.63	0.45
1:B:158:LEU:HD12	1:B:158:LEU:O	2.17	0.45
1:A:258:THR:C	1:A:260:ASP:H	2.25	0.44
1:B:247:ILE:HA	1:B:261:ASP:O	2.17	0.44
1:A:126:GLN:OE1	1:A:145:THR:HA	2.17	0.44
1:A:69:ILE:HG21	1:A:262:PHE:CD2	2.53	0.44
1:A:117:ARG:O	1:A:123:LYS:HA	2.17	0.44
1:A:158:LEU:O	1:A:158:LEU:HD12	2.17	0.44
1:B:99:GLN:O	1:B:101:ASP:N	2.51	0.44
1:A:137:ASN:O	1:A:143:HIS:HE1	2.00	0.44
1:A:187:LEU:HD11	1:A:227:HIS:HE1	1.83	0.44
1:B:55:VAL:HG12	1:B:57:ILE:CG2	2.46	0.44
1:B:187:LEU:HD11	1:B:227:HIS:HE1	1.83	0.43
1:B:258:THR:C	1:B:260:ASP:H	2.25	0.43
1:B:31:TRP:HE3	1:B:278:ALA:HB2	1.81	0.43
1:B:69:ILE:HG21	1:B:262:PHE:CD2	2.53	0.43
1:B:146:MET:CE	1:B:164:GLU:HB3	2.48	0.43
1:B:163:TYR:H	1:B:163:TYR:HD1	1.63	0.43
1:A:99:GLN:O	1:A:101:ASP:N	2.51	0.43
1:B:99:GLN:C	1:B:101:ASP:H	2.27	0.43
1:A:146:MET:CE	1:A:164:GLU:HB3	2.48	0.43
1:A:162:VAL:HG13	1:A:178:VAL:CG1	2.49	0.43
1:A:42:SER:OG	1:B:170:LYS:NZ	2.52	0.43
1:B:162:VAL:HG13	1:B:178:VAL:CG1	2.49	0.43
1:B:171:HIS:C	1:B:173:LYS:N	2.77	0.43
1:B:220:ASP:OD1	1:B:222:HIS:HD2	2.02	0.42
1:A:258:THR:C	1:A:260:ASP:N	2.77	0.42
1:B:49:ARG:HE	1:B:213:GLU:CD	2.28	0.42
1:B:133:GLN:O	1:B:137:ASN:N	2.52	0.42
1:A:171:HIS:C	1:A:173:LYS:N	2.77	0.42
1:B:232:LYS:HA	1:B:235:MET:HG3	2.01	0.42
1:B:258:THR:C	1:B:260:ASP:N	2.77	0.42
1:A:133:GLN:O	1:A:137:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HA	1:A:235:MET:HG3	2.01	0.42
1:B:64:ALA:HB3	1:B:191:PHE:CE1	2.55	0.42
1:A:49:ARG:HE	1:A:213:GLU:CD	2.28	0.42
1:A:99:GLN:C	1:A:101:ASP:H	2.27	0.42
1:A:220:ASP:OD1	1:A:222:HIS:HD2	2.02	0.42
1:B:12:ILE:HD12	1:B:231:LEU:CD1	2.31	0.42
1:B:51:ASP:O	1:B:52:ASN:HB2	2.20	0.42
1:A:45:SER:HB2	1:B:177:GLU:OE2	2.20	0.42
1:A:62:LYS:HG3	1:A:269:HIS:CE1	2.55	0.42
1:A:197:ASN:ND2	1:A:214:TYR:CD2	2.86	0.42
1:A:64:ALA:HB3	1:A:191:PHE:CE1	2.55	0.41
1:A:226:ARG:HH11	1:A:276:GLU:HG2	1.85	0.41
1:B:73:LEU:O	1:B:77:GLN:HB3	2.20	0.41
1:A:174:LEU:C	1:A:174:LEU:CD1	2.94	0.41
1:B:174:LEU:C	1:B:174:LEU:CD1	2.94	0.41
1:A:27:VAL:HG13	1:A:39:HIS:CE1	2.55	0.41
1:A:247:ILE:HG12	1:A:262:PHE:CE1	2.56	0.41
1:B:62:LYS:HG3	1:B:269:HIS:CE1	2.55	0.41
1:A:97:TRP:CG	1:A:158:LEU:HD23	2.56	0.41
1:A:51:ASP:O	1:A:52:ASN:HB2	2.20	0.41
1:A:117:ARG:NE	1:B:154:ASP:OD1	2.52	0.41
1:B:27:VAL:HG13	1:B:39:HIS:CE1	2.55	0.41
1:B:178:VAL:HG12	1:B:179:ARG:N	2.35	0.41
1:B:226:ARG:HH11	1:B:276:GLU:HG2	1.85	0.41
1:B:247:ILE:HG12	1:B:262:PHE:HD1	1.86	0.41
1:A:73:LEU:O	1:A:77:GLN:HB3	2.20	0.41
1:B:31:TRP:CH2	1:B:224:TYR:HB3	2.56	0.41
1:B:275:PHE:O	1:B:276:GLU:C	2.64	0.41
1:A:275:PHE:O	1:A:276:GLU:C	2.64	0.40
1:B:97:TRP:CG	1:B:158:LEU:HD23	2.56	0.40
1:B:99:GLN:C	1:B:101:ASP:N	2.79	0.40
1:B:197:ASN:ND2	1:B:214:TYR:CD2	2.86	0.40
1:A:31:TRP:CH2	1:A:224:TYR:HB3	2.56	0.40
1:B:31:TRP:CD2	1:B:38:ALA:HB2	2.56	0.40
1:A:61:LYS:HG3	1:A:62:LYS:N	2.36	0.40

All (8) 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:232:LYS:NZ	1:B:26:ASP:OD1[3_655]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:NZ	1:B:26:ASP:CG[3_655]	1.35	0.85
1:A:232:LYS:NZ	1:B:26:ASP:OD2[3_655]	1.60	0.60
1:B:101:ASP:CB	1:B:263:LYS:NZ[4_455]	1.72	0.48
1:A:23:GLU:OE1	1:A:171:HIS:CD2[3_655]	2.02	0.18
1:A:232:LYS:CE	1:B:26:ASP:OD1[3_655]	2.08	0.12
1:A:23:GLU:OE1	1:A:171:HIS:NE2[3_655]	2.09	0.11
1:B:101:ASP:CG	1:B:263:LYS:NZ[4_455]	2.09	0.11

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	276/278 (99%)	235 (85%)	30 (11%)	11 (4%)	2	1
1	B	276/278 (99%)	235 (85%)	30 (11%)	11 (4%)	2	1
All	All	552/556 (99%)	470 (85%)	60 (11%)	22 (4%)	2	1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	93	ILE
1	A	143	HIS
1	B	24	GLU
1	B	93	ILE
1	B	143	HIS
1	A	31	TRP
1	A	100	GLU
1	A	193	VAL
1	A	276	GLU
1	B	31	TRP
1	B	100	GLU
1	B	193	VAL

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Mol	Chain	Res	Type
1	B	276	GLU
1	A	45	SER
1	A	148	TRP
1	B	45	SER
1	B	148	TRP
1	A	3	GLN
1	A	23	GLU
1	B	3	GLN
1	B	23	GLU

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	252/253 (100%)	194 (77%)	58 (23%)	1	0
1	B	252/253 (100%)	194 (77%)	58 (23%)	1	0
All	All	504/506 (100%)	388 (77%)	116 (23%)	1	0

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	GLN
1	A	10	SER
1	A	13	LYS
1	A	21	SER
1	A	23	GLU
1	A	24	GLU
1	A	29	THR
1	A	30	LYS
1	A	32	ASP
1	A	34	ASP
1	A	40	THR
1	A	42	SER
1	A	46	LYS

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Mol	Chain	Res	Type
1	A	55	VAL
1	A	57	ILE
1	A	61	LYS
1	A	62	LYS
1	A	66	LYS
1	A	67	THR
1	A	78	LEU
1	A	96	GLN
1	A	100	GLU
1	A	104	ILE
1	A	117	ARG
1	A	119	LEU
1	A	123	LYS
1	A	124	VAL
1	A	135	LYS
1	A	137	ASN
1	A	139	SER
1	A	142	ARG
1	A	145	THR
1	A	154	ASP
1	A	156	MET
1	A	158	LEU
1	A	159	THR
1	A	164	GLU
1	A	166	GLN
1	A	173	LYS
1	A	174	LEU
1	A	181	ARG
1	A	183	ASN
1	A	187	LEU
1	A	203	ILE
1	A	206	VAL
1	A	211	LEU
1	A	213	GLU
1	A	221	CYS
1	A	225	THR
1	A	232	LYS
1	A	236	GLU
1	A	241	GLU
1	A	244	GLU
1	A	263	LYS
1	A	268	LYS

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	274	LEU
1	B	2	THR
1	B	3	GLN
1	B	10	SER
1	B	13	LYS
1	B	21	SER
1	B	23	GLU
1	B	24	GLU
1	B	29	THR
1	B	30	LYS
1	B	32	ASP
1	B	34	ASP
1	B	40	THR
1	B	42	SER
1	B	46	LYS
1	B	55	VAL
1	B	57	ILE
1	B	61	LYS
1	B	62	LYS
1	B	66	LYS
1	B	67	THR
1	B	78	LEU
1	B	96	GLN
1	B	100	GLU
1	B	104	ILE
1	B	117	ARG
1	B	119	LEU
1	B	123	LYS
1	B	124	VAL
1	B	135	LYS
1	B	137	ASN
1	B	139	SER
1	B	142	ARG
1	B	145	THR
1	B	154	ASP
1	B	156	MET
1	B	158	LEU
1	B	159	THR
1	B	164	GLU
1	B	166	GLN
1	B	173	LYS

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Mol	Chain	Res	Type
1	B	174	LEU
1	B	181	ARG
1	B	183	ASN
1	B	187	LEU
1	B	203	ILE
1	B	206	VAL
1	B	211	LEU
1	B	213	GLU
1	B	221	CYS
1	B	225	THR
1	B	232	LYS
1	B	236	GLU
1	B	241	GLU
1	B	244	GLU
1	B	263	LYS
1	B	268	LYS
1	B	273	LEU
1	B	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	ASN
1	A	87	ASN
1	A	137	ASN
1	A	183	ASN
1	A	189	ASN
1	A	192	ASN
1	A	195	GLN
1	A	222	HIS
1	A	266	ASN
1	B	3	GLN
1	B	9	ASN
1	B	87	ASN
1	B	111	GLN
1	B	137	ASN
1	B	183	ASN
1	B	189	ASN
1	B	192	ASN
1	B	195	GLN
1	B	222	HIS

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Mol	Chain	Res	Type
1	B	266	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

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.