



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 1SRY / pdb_00001sry
Title : REFINED CRYSTAL STRUCTURE OF THE SERYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS AT 2.5 ANGSTROMS RESOLUTION
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Deposited on : 1993-08-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

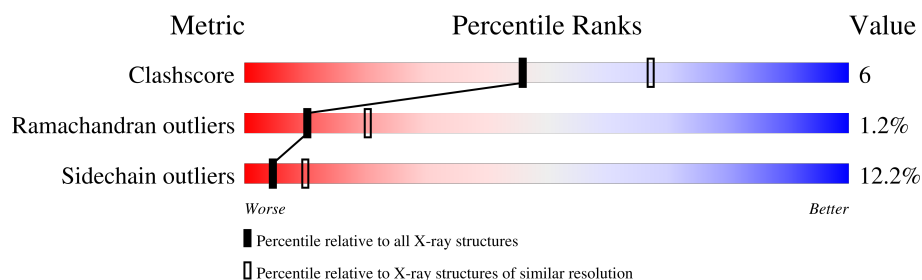
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	421	 72% 23% 5% •
1	B	421	 68% 24% 6% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6936 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 SERYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3373	2143	606	613	11			
1	B	421	Total	C	N	O	S	0	0	0
			3373	2143	606	613	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	conflict	UNP P34945
B	208	TYR	THR	conflict	UNP P34945

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	96	Total	O	0	0
			96	96		

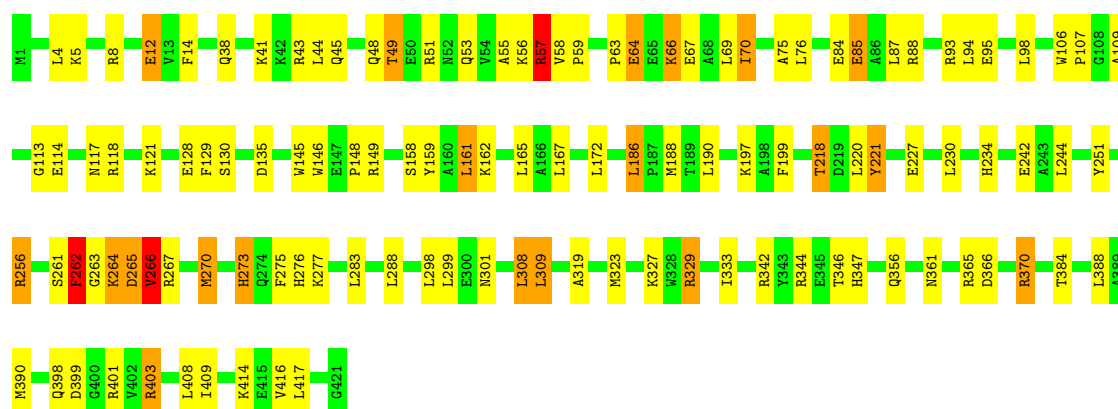
3 Residue-property plots

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.

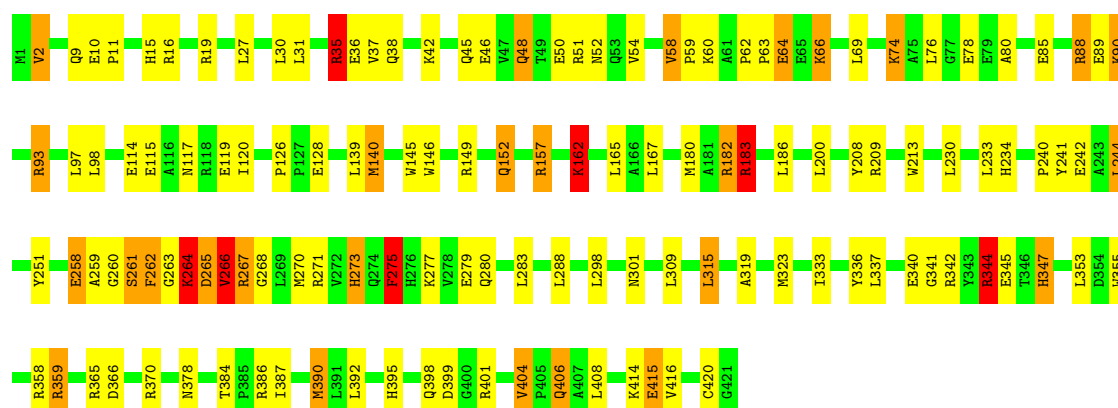
• Molecule 1: SERYL-tRNA SYNTHETASE

Chain A: 



• Molecule 1: SERYL-tRNA SYNTHETASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.03Å 127.46Å 63.37Å 90.00° 108.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GROMOS	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6936	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	1.06	3/3448 (0.1%)	1.67	33/4667 (0.7%)
1	B	1.06	3/3448 (0.1%)	1.71	39/4667 (0.8%)
All	All	1.06	6/6896 (0.1%)	1.69	72/9334 (0.8%)

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	23
1	B	0	31
All	All	0	54

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	HIS	CG-ND1	-5.32	1.32	1.38
1	A	276	HIS	CG-ND1	-5.22	1.32	1.38
1	A	145	TRP	NE1-CE2	-5.18	1.31	1.37
1	B	273	HIS	CG-ND1	-5.16	1.32	1.38
1	B	395	HIS	CD2-NE2	-5.14	1.32	1.37
1	B	145	TRP	NE1-CE2	-5.01	1.31	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ASP	CA-CB-CG	-9.41	103.19	112.60
1	A	323	MET	N-CA-C	7.74	120.39	111.11
1	B	262	PHE	CA-CB-CG	7.30	121.10	113.80
1	B	262	PHE	N-CA-C	7.09	119.46	110.24
1	A	403	ARG	N-CA-CB	-6.80	100.38	110.17
1	B	404	VAL	CB-CA-C	6.77	117.70	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	PHE	CA-CB-CG	-6.64	107.16	113.80
1	B	58	VAL	CB-CA-C	6.60	123.38	111.36
1	A	121	LYS	N-CA-CB	-6.54	100.84	111.24
1	A	409	ILE	CA-C-O	-6.38	113.43	118.85
1	A	129	PHE	CA-CB-CG	-6.29	107.51	113.80
1	B	265	ASP	N-CA-C	6.22	124.05	110.80
1	A	118	ARG	N-CA-CB	-6.22	101.01	110.77
1	B	273	HIS	N-CA-C	6.20	118.03	111.28
1	A	135	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	409	ILE	O-C-N	6.13	124.42	120.07
1	A	114	GLU	N-CA-CB	-6.07	100.56	110.14
1	B	273	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	301	ASN	CA-C-N	5.93	128.16	120.44
1	A	301	ASN	C-N-CA	5.93	128.16	120.44
1	B	15	HIS	CA-CB-CG	-5.84	107.96	113.80
1	B	89	GLU	N-CA-CB	-5.81	99.84	109.72
1	B	93	ARG	N-CA-CB	-5.81	101.57	110.12
1	A	361	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	B	344	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	B	234	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	93	ARG	N-CA-CB	-5.75	101.67	110.12
1	B	270	MET	N-CA-C	5.73	117.20	111.07
1	B	140	MET	CA-C-N	5.70	128.71	120.79
1	B	140	MET	C-N-CA	5.70	128.71	120.79
1	A	4	LEU	N-CA-C	5.68	118.20	111.33
1	A	370	ARG	N-CA-CB	5.65	119.38	110.23
1	A	308	LEU	N-CA-CB	-5.63	101.54	110.22
1	B	162	LYS	N-CA-CB	-5.59	101.60	111.39
1	B	344	ARG	N-CA-CB	-5.59	101.12	110.80
1	B	277	LYS	N-CA-CB	-5.59	101.42	110.81
1	A	309	LEU	N-CA-CB	-5.55	101.75	110.46
1	B	275	PHE	CA-CB-CG	5.54	119.34	113.80
1	B	51	ARG	N-CA-CB	-5.53	102.00	110.12
1	B	152	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	B	35	ARG	CD-NE-CZ	5.50	132.11	124.40
1	B	183	ARG	CD-NE-CZ	5.50	132.10	124.40
1	B	38	GLN	N-CA-C	5.48	117.33	111.36
1	A	49	THR	CA-CB-CG2	5.47	119.79	110.50
1	B	366	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	234	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	B	2	VAL	N-CA-CB	-5.40	102.49	112.43
1	A	266	VAL	CB-CA-C	5.39	120.14	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLU	N-CA-CB	-5.36	102.23	110.01
1	B	90	LYS	N-CA-C	5.36	116.80	111.07
1	B	42	LYS	CB-CA-C	5.34	119.23	110.95
1	B	119	GLU	CA-C-N	5.34	127.40	120.88
1	B	119	GLU	C-N-CA	5.34	127.40	120.88
1	A	299	LEU	N-CA-CB	-5.30	102.29	110.13
1	B	42	LYS	N-CA-CB	-5.29	102.31	109.98
1	A	93	ARG	CB-CG-CD	-5.24	99.24	111.30
1	B	337	LEU	CA-C-N	5.24	124.69	119.24
1	B	337	LEU	C-N-CA	5.24	124.69	119.24
1	A	113	GLY	CA-C-N	5.19	127.95	120.38
1	A	113	GLY	C-N-CA	5.19	127.95	120.38
1	B	244	LEU	N-CA-CB	-5.16	102.87	110.14
1	B	415	GLU	N-CA-CB	-5.16	102.40	110.44
1	A	63	PRO	O-C-N	5.14	127.73	122.18
1	B	347	HIS	CB-CG-CD2	-5.13	124.52	131.20
1	B	323	MET	N-CA-CB	-5.11	102.60	110.01
1	A	264	LYS	CA-C-O	5.09	125.74	120.40
1	B	340	GLU	N-CA-CB	-5.08	102.86	110.73
1	A	12	GLU	CA-C-N	5.07	126.95	120.56
1	A	12	GLU	C-N-CA	5.07	126.95	120.56
1	A	75	ALA	CA-C-N	5.07	127.07	120.28
1	A	75	ALA	C-N-CA	5.07	127.07	120.28
1	A	38	GLN	OE1-CD-NE2	-5.06	117.54	122.60

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PRO	Mainchain
1	A	12	GLU	Mainchain
1	A	221	TYR	Sidechain
1	A	251	TYR	Sidechain
1	A	262	PHE	Mainchain,Peptide,Sidechain
1	A	265	ASP	Mainchain,Peptide
1	A	267	ARG	Sidechain
1	A	273	HIS	Sidechain
1	A	283	LEU	Mainchain
1	A	327	LYS	Mainchain
1	A	342	ARG	Sidechain
1	A	356	GLN	Mainchain
1	A	365	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	370	ARG	Sidechain
1	A	398	GLN	Mainchain
1	A	403	ARG	Sidechain
1	A	51	ARG	Mainchain
1	A	57	ARG	Sidechain
1	A	64	GLU	Mainchain
1	A	8	ARG	Sidechain
1	B	120	ILE	Mainchain
1	B	149	ARG	Sidechain
1	B	157	ARG	Sidechain
1	B	162	LYS	Mainchain
1	B	182	ARG	Sidechain
1	B	183	ARG	Sidechain
1	B	19	ARG	Mainchain
1	B	208	TYR	Sidechain
1	B	209	ARG	Sidechain
1	B	240	PRO	Mainchain
1	B	251	TYR	Sidechain
1	B	258	GLU	Peptide
1	B	259	ALA	Mainchain
1	B	264	LYS	Peptide
1	B	266	VAL	Peptide
1	B	267	ARG	Peptide
1	B	342	ARG	Sidechain
1	B	344	ARG	Sidechain
1	B	35	ARG	Sidechain
1	B	358	ARG	Sidechain
1	B	359	ARG	Sidechain
1	B	37	VAL	Mainchain
1	B	386	ARG	Sidechain
1	B	399	ASP	Mainchain
1	B	401	ARG	Sidechain
1	B	45	GLN	Mainchain
1	B	48	GLN	Mainchain
1	B	52	ASN	Mainchain
1	B	60	LYS	Peptide
1	B	80	ALA	Mainchain
1	B	88	ARG	Sidechain

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	3373	0	3394	39	1
1	B	3373	0	3394	43	1
2	A	94	0	0	5	0
2	B	96	0	0	5	0
All	All	6936	0	6788	78	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 6.

All (78) 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:140:MET:HE2	1:B:146:TRP:HB3	1.50	0.92
1:B:267:ARG:HD3	1:B:268:GLY:H	1.46	0.79
1:A:186:LEU:HD21	1:B:162:LYS:HG3	1.70	0.74
1:A:53:GLN:HB3	1:A:57:ARG:NH1	2.06	0.71
1:A:85:GLU:HA	1:A:88:ARG:HE	1.56	0.70
1:B:11:PRO:HB2	1:B:27:LEU:HD21	1.75	0.69
1:B:157:ARG:NH2	1:B:271:ARG:HD2	2.09	0.68
1:A:188:MET:HE2	1:A:190:LEU:HD21	1.79	0.65
1:A:266:VAL:HG21	1:A:344:ARG:HH21	1.64	0.63
1:B:180:MET:HE2	1:B:280:GLN:HG2	1.81	0.63
1:B:157:ARG:HH21	1:B:271:ARG:HD2	1.65	0.61
1:B:117:ASN:ND2	1:B:319:ALA:H	1.99	0.61
1:A:158:SER:HA	2:B:429:HOH:O	2.00	0.60
1:A:266:VAL:HG13	1:A:270:MET:HB2	1.83	0.60
1:B:241:TYR:HB2	1:B:365:ARG:O	2.02	0.60
1:A:218:THR:HG23	1:A:220:LEU:H	1.68	0.59
1:B:157:ARG:HH21	1:B:262:PHE:HB2	1.68	0.59
1:B:267:ARG:CD	1:B:268:GLY:H	2.14	0.58
1:A:399:ASP:OD1	1:A:401:ARG:HG2	2.02	0.58
1:A:117:ASN:ND2	1:A:319:ALA:H	2.01	0.58
1:B:183:ARG:HH11	1:B:301:ASN:ND2	2.02	0.58
1:B:54:VAL:O	1:B:58:VAL:HG23	2.04	0.57
1:B:126:PRO:HD3	2:B:512:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HD21	2:B:515:HOH:O	2.05	0.56
1:A:275:PHE:HB2	1:A:384:THR:O	2.08	0.53
1:A:55:ALA:O	1:A:59:PRO:HD2	2.09	0.52
1:A:261:SER:O	1:A:262:PHE:HB2	2.09	0.52
1:A:58:VAL:HG22	1:A:69:LEU:HB3	1.92	0.52
1:B:66:LYS:NZ	1:B:66:LYS:HB2	2.24	0.52
1:A:106:TRP:CD1	1:A:329:ARG:HG2	2.46	0.51
1:A:218:THR:CG2	1:A:220:LEU:H	2.23	0.51
1:B:63:PRO:HA	1:B:66:LYS:HG2	1.93	0.51
1:A:333:ILE:HB	1:A:347:HIS:HB2	1.93	0.51
1:A:94:LEU:O	1:A:98:LEU:HD23	2.12	0.50
1:A:66:LYS:O	1:A:70:ILE:HG22	2.12	0.50
1:B:93:ARG:O	1:B:97:LEU:HD13	2.12	0.50
1:B:275:PHE:HB2	1:B:384:THR:O	2.11	0.50
1:B:392:LEU:HD11	2:B:515:HOH:O	2.11	0.49
1:B:58:VAL:HG12	1:B:59:PRO:HD3	1.95	0.49
1:B:27:LEU:O	1:B:30:LEU:HB3	2.13	0.48
1:A:277:LYS:HB3	2:A:437:HOH:O	2.13	0.48
1:B:263:GLY:O	1:B:264:LYS:HB2	2.13	0.48
1:B:344:ARG:HB3	1:B:390:MET:CE	2.43	0.48
1:A:44:LEU:HD11	1:A:84:GLU:HG3	1.95	0.48
1:A:388:LEU:HG	2:A:511:HOH:O	2.13	0.48
1:A:401:ARG:HB2	1:A:417:LEU:O	2.14	0.48
1:A:414:LYS:HD3	1:A:416:VAL:O	2.14	0.48
1:A:165:LEU:HD11	1:A:388:LEU:HD22	1.95	0.48
1:B:74:LYS:O	1:B:78:GLU:HG2	2.14	0.47
1:B:62:PRO:HB2	1:B:64:GLU:HG3	1.96	0.47
1:B:262:PHE:HB3	1:B:266:VAL:N	2.29	0.47
1:B:200:LEU:O	1:B:359:ARG:HD3	2.15	0.47
1:A:172:LEU:HD13	2:A:511:HOH:O	2.15	0.47
1:A:41:LYS:HG2	1:A:87:LEU:HD21	1.98	0.46
1:A:106:TRP:CD1	1:A:109:ALA:HB2	2.51	0.46
1:B:414:LYS:HD3	1:B:416:VAL:O	2.14	0.46
1:A:149:ARG:HD3	1:B:233:LEU:O	2.16	0.46
1:A:44:LEU:O	1:A:48:GLN:HG2	2.17	0.46
1:A:159:TYR:HD2	1:A:161:LEU:HD13	1.81	0.45
2:A:501:HOH:O	1:B:273:HIS:HB2	2.16	0.45
1:A:186:LEU:HD11	1:B:420:CYS:SG	2.57	0.45
1:B:140:MET:HE2	1:B:146:TRP:CB	2.36	0.45
1:B:344:ARG:HB3	1:B:390:MET:HE2	1.98	0.45
1:B:355:TRP:O	1:B:359:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HB3	1:B:336:TYR:CE2	2.53	0.44
1:A:172:LEU:CD1	2:A:511:HOH:O	2.65	0.44
1:A:256:ARG:HB3	1:A:256:ARG:HH11	1.83	0.44
1:A:346:THR:CG2	1:A:390:MET:HE3	2.49	0.43
1:A:199:PHE:CE2	1:A:221:TYR:HB2	2.54	0.43
1:A:262:PHE:CD2	1:A:263:GLY:N	2.85	0.43
1:A:146:TRP:O	1:A:148:PRO:HD3	2.20	0.42
1:B:183:ARG:HH11	1:B:301:ASN:HD22	1.68	0.42
1:B:333:ILE:HB	1:B:347:HIS:HB2	2.01	0.42
1:B:420:CYS:HB2	2:B:437:HOH:O	2.19	0.41
1:B:336:TYR:OH	1:B:341:GLY:HA2	2.20	0.41
1:B:315:LEU:HD22	1:B:333:ILE:HG12	2.03	0.41
1:B:30:LEU:HD13	1:B:97:LEU:HB3	2.03	0.40
1:A:162:LYS:HE2	1:B:186:LEU:HD21	2.03	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)
1:A:130:SER:OG	1:B:64:GLU:OE2[1_656]	1.95	0.25

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	419/421 (100%)	391 (93%)	25 (6%)	3 (1%)	18	34
1	B	419/421 (100%)	394 (94%)	18 (4%)	7 (2%)	7	13
All	All	838/842 (100%)	785 (94%)	43 (5%)	10 (1%)	10	20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	PHE
1	B	264	LYS
1	B	266	VAL
1	A	64	GLU
1	A	265	ASP
1	B	265	ASP
1	B	260	GLY
1	B	406	GLN
1	B	261	SER
1	B	10	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	347/347 (100%)	314 (90%)	33 (10%)	8	17
1	B	347/347 (100%)	295 (85%)	52 (15%)	3	6
All	All	694/694 (100%)	609 (88%)	85 (12%)	5	10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	43	ARG
1	A	45	GLN
1	A	49	THR
1	A	56	LYS
1	A	57	ARG
1	A	66	LYS
1	A	67	GLU
1	A	70	ILE
1	A	76	LEU
1	A	95	GLU
1	A	128	GLU
1	A	161	LEU
1	A	167	LEU

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Mol	Chain	Res	Type
1	A	186	LEU
1	A	197	LYS
1	A	218	THR
1	A	227	GLU
1	A	230	LEU
1	A	242	GLU
1	A	244	LEU
1	A	256	ARG
1	A	262	PHE
1	A	264	LYS
1	A	266	VAL
1	A	270	MET
1	A	288	LEU
1	A	298	LEU
1	A	308	LEU
1	A	309	LEU
1	A	329	ARG
1	A	366	ASP
1	A	408	LEU
1	B	2	VAL
1	B	9	GLN
1	B	16	ARG
1	B	31	LEU
1	B	35	ARG
1	B	36	GLU
1	B	46	GLU
1	B	48	GLN
1	B	50	GLU
1	B	64	GLU
1	B	66	LYS
1	B	69	LEU
1	B	74	LYS
1	B	76	LEU
1	B	85	GLU
1	B	88	ARG
1	B	90	LYS
1	B	98	LEU
1	B	114	GLU
1	B	115	GLU
1	B	128	GLU
1	B	139	LEU
1	B	152	GLN

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Mol	Chain	Res	Type
1	B	167	LEU
1	B	182	ARG
1	B	183	ARG
1	B	213	TRP
1	B	230	LEU
1	B	242	GLU
1	B	244	LEU
1	B	258	GLU
1	B	261	SER
1	B	264	LYS
1	B	275	PHE
1	B	279	GLU
1	B	283	LEU
1	B	288	LEU
1	B	298	LEU
1	B	309	LEU
1	B	315	LEU
1	B	344	ARG
1	B	345	GLU
1	B	353	LEU
1	B	370	ARG
1	B	378	ASN
1	B	387	ILE
1	B	390	MET
1	B	398	GLN
1	B	404	VAL
1	B	406	GLN
1	B	408	LEU
1	B	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	117	ASN
1	A	280	GLN
1	A	296	GLN
1	A	301	ASN
1	A	356	GLN
1	A	361	ASN
1	A	379	ASN
1	B	117	ASN

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Mol	Chain	Res	Type
1	B	136	HIS
1	B	152	GLN
1	B	211	GLN
1	B	274	GLN
1	B	276	HIS
1	B	280	GLN
1	B	296	GLN
1	B	301	ASN
1	B	356	GLN
1	B	361	ASN
1	B	378	ASN
1	B	394	ASN
1	B	398	GLN
1	B	406	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

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.