



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:14 PM GMT

PDB ID : 1SRY
Title : REFINED CRYSTAL STRUCTURE OF THE SERYL-TRNA SYN-
THETASE FROM THERMUS THERMOPHILUS AT 2.5 ANGSTROMS
RESOLUTION
Authors : Fujinaga, M.; Berthet-Colominas, C.; Cusack, S.
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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

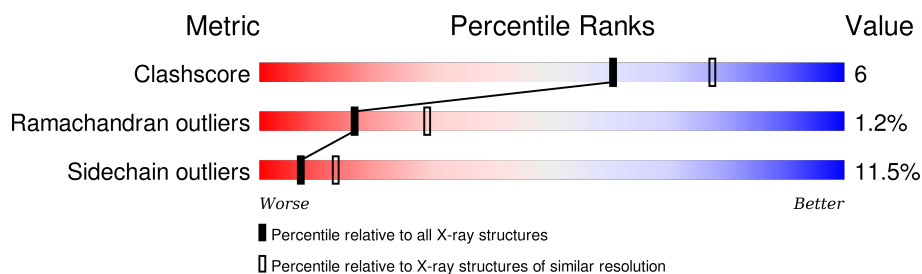
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	 72% 22% 5% •
1	B	421	 68% 23% 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.

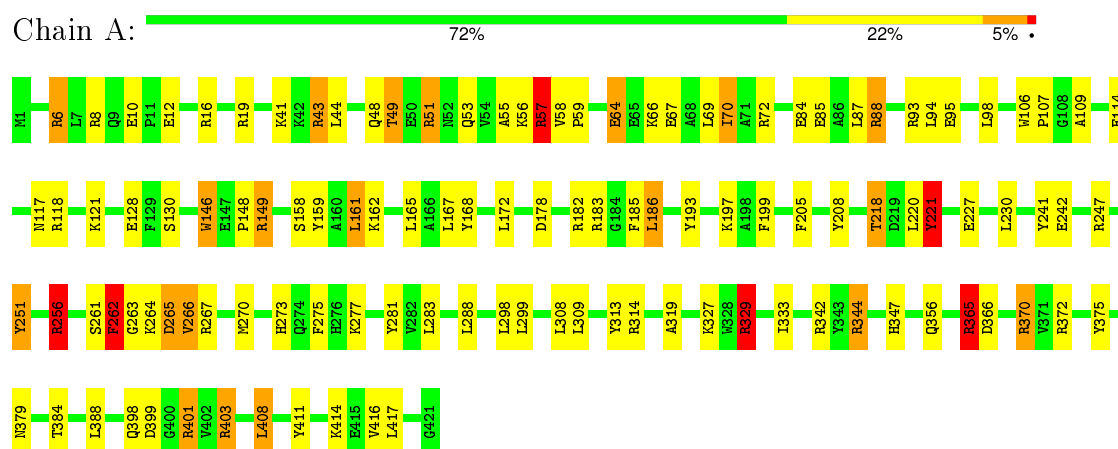
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	96	Total	O	0	0
			96	96		

3 Residue-property plots

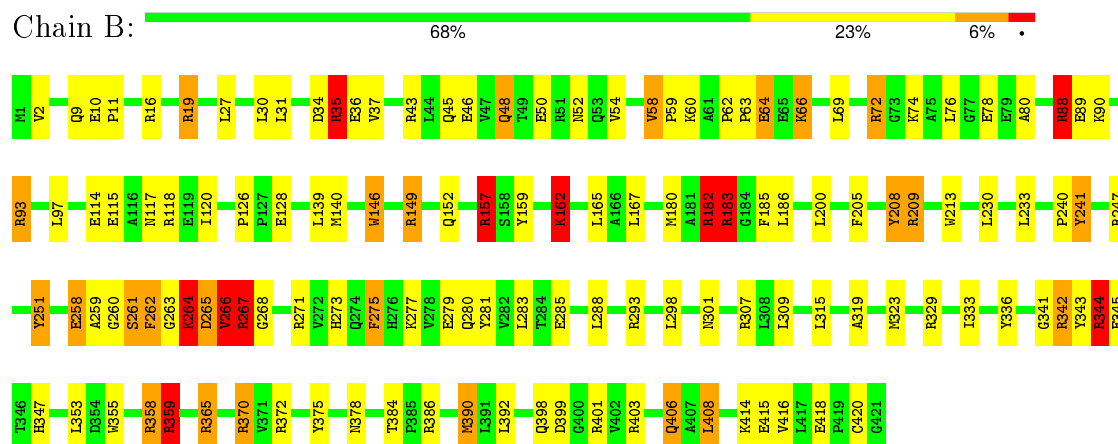
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: SERYL-tRNA SYNTHETASE



• Molecule 1: SERYL-tRNA SYNTHETASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.84	0/3448	1.51	51/4667 (1.1%)
1	B	0.83	0/3448	1.55	54/4667 (1.2%)
All	All	0.83	0/6896	1.53	105/9334 (1.1%)

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

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	A	256	ARG	NE-CZ-NH1	10.77	125.68	120.30
1	B	35	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	A	365	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	B	183	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	370	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	262	PHE	CB-CG-CD1	-9.98	113.81	120.80
1	B	358	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	B	358	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	A	118	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	A	72	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	343	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	B	183	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	A	247	ARG	NE-CZ-NH2	-8.68	115.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	365	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	375	TYR	CB-CG-CD2	-8.53	115.88	121.00
1	A	262	PHE	CB-CG-CD2	-8.46	114.88	120.80
1	A	344	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	183	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	193	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	A	149	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	372	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	403	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	267	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	118	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	157	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	281	TYR	CB-CG-CD1	-7.54	116.47	121.00
1	B	159	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	B	241	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	A	205	PHE	CB-CG-CD2	-7.41	115.61	120.80
1	A	375	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	B	342	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	93	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	314	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	241	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	A	313	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	149	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	372	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	6	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	B	372	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	403	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	408	LEU	CA-CB-CG	-6.57	100.19	115.30
1	B	267	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	359	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	88	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	401	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	408	LEU	CA-CB-CG	-6.41	100.56	115.30
1	A	329	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	344	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	307	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	58	VAL	CB-CA-C	6.30	123.38	111.40
1	A	281	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	B	247	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	262	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	B	43	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	B	19	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	35	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	183	ARG	CD-NE-CZ	6.07	132.10	123.60
1	A	251	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	B	89	GLU	N-CA-CB	-5.98	99.84	110.60
1	A	411	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	19	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	57	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	403	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	205	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	A	370	ARG	NH1-CZ-NH2	-5.74	113.09	119.40
1	B	251	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	B	208	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	403	ARG	N-CA-CB	-5.68	100.38	110.60
1	B	72	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	16	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	93	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	329	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	114	GLU	N-CA-CB	-5.58	100.56	110.60
1	A	221	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	A	88	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	365	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	35	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	B	370	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	209	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	35	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	57	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	285	GLU	OE1-CD-OE2	5.43	129.81	123.30
1	A	121	LYS	N-CA-CB	-5.42	100.84	110.60
1	A	185	PHE	CB-CG-CD2	-5.41	117.02	120.80
1	A	329	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
1	A	118	ARG	N-CA-CB	-5.33	101.01	110.60
1	A	299	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	A	208	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	49	THR	CA-CB-CG2	5.28	119.79	112.40
1	B	344	ARG	N-CA-CB	-5.27	101.12	110.60
1	A	51	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	185	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	B	293	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	149	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	277	LYS	N-CA-CB	-5.10	101.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	323	MET	CG-SD-CE	-5.09	92.05	100.20
1	B	34	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	93	ARG	N-CA-CB	-5.01	101.57	110.60
1	A	178	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	183	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	B	162	LYS	N-CA-CB	-5.00	101.60	110.60

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	Sidechain,Mainchain,Peptide
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
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

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Mol	Chain	Res	Type	Group
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	37	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	76	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 (76) 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:267:ARG:HD3	1:B:268:GLY:H	1.46	0.79
1:B:180:MET:HE2	1:B:280:GLN:HG2	1.69	0.75
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:266:VAL:HG21	1:A:344:ARG:HH21	1.64	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:266:VAL:HG13	1:A:270:MET:HB2	1.83	0.60
1:A:158:SER:HA	2:B:429:HOH:O	2.00	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:B:183:ARG:HH11	1:B:301:ASN:ND2	2.02	0.58
1:A:117:ASN:ND2	1:A:319:ALA:H	2.01	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
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:B:140:MET:CE	1:B:146:TRP:HB3	2.38	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:HB2	1:B:66:LYS:NZ	2.24	0.52
1:B:140:MET:HE2	1:B:146:TRP:HB3	1.91	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:388:LEU:HG	2:A:511:HOH:O	2.13	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:262:PHE:HB3	1:B:266:VAL:N	2.29	0.47
1:B:62:PRO:HB2	1:B:64:GLU:HG3	1.96	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: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:41:LYS:HG2	1:A:87:LEU:HD21	1.98	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:355:TRP:O	1:B:359:ARG:HG2	2.17	0.45
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:HH11	1:A:256:ARG:HB3	1.83	0.44
1:B:414:LYS:HZ1	1:B:418:GLU:HG3	1.82	0.43
1:A:262:PHE:CD2	1:A:263:GLY:N	2.85	0.43
1:A:199:PHE:CE2	1:A:221:TYR:HB2	2.54	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 [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	419/421 (100%)	391 (93%)	25 (6%)	3 (1%)	26	46
1	B	419/421 (100%)	394 (94%)	18 (4%)	7 (2%)	11	19
All	All	838/842 (100%)	785 (94%)	43 (5%)	10 (1%)	16	29

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 [i](#)

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%)	315 (91%)	32 (9%)	11	21
1	B	347/347 (100%)	299 (86%)	48 (14%)	4	8
All	All	694/694 (100%)	614 (88%)	80 (12%)	7	13

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	10	GLU
1	A	43	ARG
1	A	49	THR
1	A	56	LYS
1	A	67	GLU
1	A	70	ILE
1	A	95	GLU
1	A	128	GLU
1	A	146	TRP
1	A	161	LEU
1	A	167	LEU
1	A	182	ARG
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	256	ARG
1	A	262	PHE
1	A	264	LYS
1	A	266	VAL
1	A	288	LEU
1	A	298	LEU
1	A	308	LEU
1	A	309	LEU
1	A	329	ARG
1	A	365	ARG
1	A	366	ASP
1	A	379	ASN
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

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Mol	Chain	Res	Type
1	B	66	LYS
1	B	69	LEU
1	B	72	ARG
1	B	76	LEU
1	B	88	ARG
1	B	90	LYS
1	B	114	GLU
1	B	115	GLU
1	B	128	GLU
1	B	139	LEU
1	B	146	TRP
1	B	152	GLN
1	B	167	LEU
1	B	182	ARG
1	B	183	ARG
1	B	213	TRP
1	B	230	LEU
1	B	258	GLU
1	B	261	SER
1	B	264	LYS
1	B	265	ASP
1	B	267	ARG
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	344	ARG
1	B	345	GLU
1	B	353	LEU
1	B	370	ARG
1	B	378	ASN
1	B	390	MET
1	B	398	GLN
1	B	406	GLN
1	B	408	LEU
1	B	415	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
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
1	B	136	HIS
1	B	231	ASN
1	B	274	GLN
1	B	276	HIS
1	B	280	GLN
1	B	296	GLN
1	B	301	ASN
1	B	361	ASN
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 carbohydrates 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 ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.