



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:46 PM GMT

PDB ID : 1VBN
Title : Escherichia coli tyrosyl-tRNA synthetase mutant complexed with Tyr-AMS
Authors : Kobayashi, T.; Sakamoto, K.; Takimura, T.; Kamata, K.; Sekine, R.;
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Deposited on : 2004-02-27
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

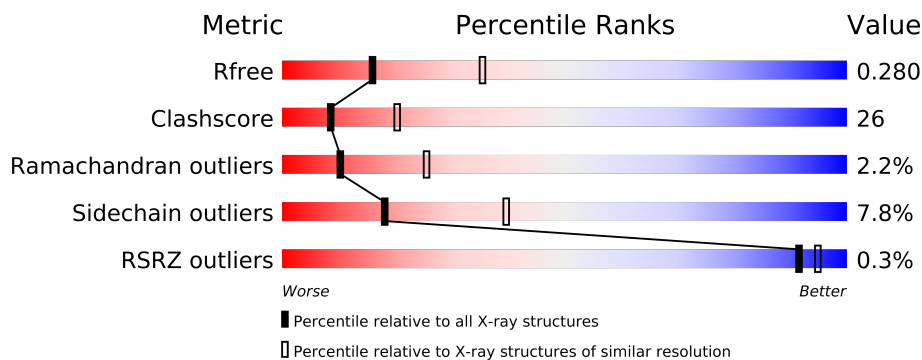
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	318	
1	B	318	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5207 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

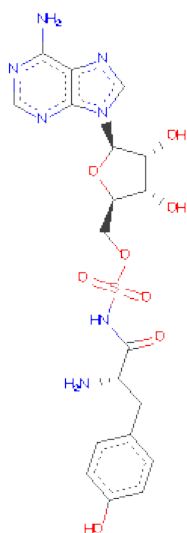
- Molecule 1 is a protein called Tyrosyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2511	1598	435	470	8			
1	B	318	Total	C	N	O	S	0	0	0
			2511	1598	435	470	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	VAL	TYR	ENGINEERED	UNP P00951
A	195	CYS	GLN	ENGINEERED	UNP P00951
B	37	VAL	TYR	ENGINEERED	UNP P00951
B	195	CYS	GLN	ENGINEERED	UNP P00951

- Molecule 2 is 5'-O-[N-(L-TYROSYL)SULFAMOYL]ADENOSINE (three-letter code: YSA) (formula: C₁₉H₂₃N₇O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	19	7	8	1		
2	B	1	Total	C	N	O	S	0	0
			35	19	7	8	1		

- Molecule 3 is water.

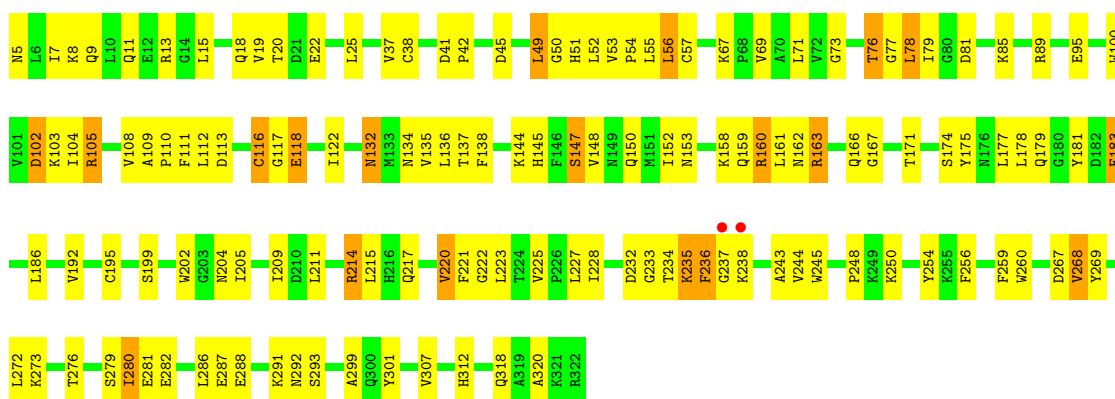
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	56	Total	O	0	0
			56	56		

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.

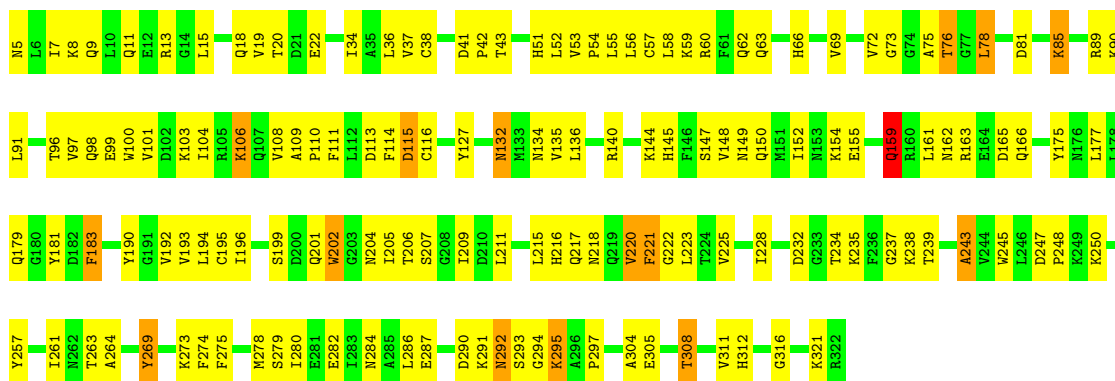
• Molecule 1: Tyrosyl-tRNA synthetase

Chain A: 



• Molecule 1: Tyrosyl-tRNA synthetase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.63Å 83.63Å 183.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.73 – 2.70 46.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (46.73-2.70) 95.3 (46.73-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.283 0.217 , 0.280	Depositor DCC
R_{free} test set	1982 reflections (9.85%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.3	EDS
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 20115 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.5419e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YSA

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	0.40	0/2563	0.63	0/3464
1	B	0.40	0/2563	0.63	0/3464
All	All	0.40	0/5126	0.63	0/6928

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	269	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2478	136	0
1	B	2511	0	2478	126	0
2	A	35	0	22	5	0
2	B	35	0	22	6	0
3	A	59	0	0	4	0
3	B	56	0	0	1	0
All	All	5207	0	5000	260	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (260) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:LYS:HE3	1:A:122:ILE:HD11	1.35	1.07
1:A:134:ASN:HD21	1:A:136:LEU:HB2	1.30	0.96
1:B:152:ILE:HG23	1:B:161:LEU:HD13	1.52	0.89
1:B:53:VAL:HB	1:B:54:PRO:HD3	1.56	0.88
1:A:37:VAL:HG23	1:A:192:VAL:HG11	1.55	0.87
1:B:290:ASP:OD1	1:B:297:PRO:HA	1.76	0.86
1:A:166:GLN:HE21	1:A:167:GLY:H	1.22	0.85
1:B:97:VAL:O	1:B:101:VAL:HG23	1.77	0.85
1:A:235:LYS:HD2	1:A:235:LYS:H	1.42	0.85
1:A:199:SER:HB3	1:A:227:LEU:HD13	1.60	0.84
1:A:102:ASP:HA	1:A:105:ARG:HD2	1.63	0.80
1:A:53:VAL:HB	1:A:54:PRO:HD3	1.63	0.79
1:A:159:GLN:HG2	3:A:1046:HOH:O	1.82	0.79
1:A:67:LYS:HE3	1:A:122:ILE:CD1	2.12	0.77
1:A:235:LYS:HG2	1:A:236:PHE:N	2.01	0.76
1:A:109:ALA:HB3	1:A:110:PRO:HD3	1.66	0.75
1:A:67:LYS:CE	1:A:122:ILE:HD11	2.16	0.74
1:B:13:ARG:HB2	1:B:273:LYS:HB3	1.68	0.74
1:B:51:HIS:CD2	2:B:1002:YSA:H5'2	2.23	0.74
1:A:166:GLN:NE2	1:A:167:GLY:H	1.84	0.73
1:A:248:PRO:HG3	1:A:312:HIS:CE1	2.24	0.73
1:A:37:VAL:HG23	1:A:192:VAL:CG1	2.19	0.73
1:B:154:LYS:HE3	1:B:207:SER:OG	1.88	0.71
1:B:179:GLN:HG3	2:B:1002:YSA:CZ	2.22	0.70
1:A:134:ASN:ND2	1:A:137:THR:H	1.90	0.70
1:A:37:VAL:HG22	1:A:69:VAL:HB	1.72	0.69
1:A:19:VAL:HG11	1:A:22:GLU:HB2	1.74	0.69
1:A:195:CYS:SG	1:A:205:ILE:HD12	2.32	0.68
1:A:235:LYS:HG2	1:A:236:PHE:H	1.57	0.68
1:B:279:SER:OG	1:B:282:GLU:HG2	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:VAL:CG2	1:A:192:VAL:HG11	2.24	0.67
1:A:179:GLN:NE2	1:A:204:ASN:HB3	2.09	0.67
1:A:85:LYS:O	1:A:160:ARG:HD3	1.94	0.67
1:B:248:PRO:HG3	1:B:312:HIS:CE1	2.29	0.67
1:B:237:GLY:O	1:B:243:ALA:HA	1.93	0.67
1:A:209:ILE:HG23	1:A:220:VAL:HG12	1.76	0.66
1:A:15:LEU:O	1:A:225:VAL:HG12	1.96	0.66
1:A:49:LEU:HD11	1:A:260:TRP:CH2	2.31	0.66
1:A:45:ASP:HB2	1:A:103:LYS:HD2	1.78	0.65
1:B:247:ASP:HB3	1:B:250:LYS:HG3	1.78	0.65
1:A:134:ASN:ND2	1:A:136:LEU:HB2	2.08	0.65
1:B:51:HIS:HD2	2:B:1002:YSA:H5'2	1.59	0.64
1:B:19:VAL:HG11	1:B:22:GLU:HB2	1.80	0.64
1:A:235:LYS:HD2	1:A:235:LYS:N	2.11	0.63
1:B:152:ILE:HG23	1:B:161:LEU:CD1	2.25	0.63
1:B:148:VAL:O	1:B:152:ILE:HG12	1.98	0.63
1:B:196:ILE:HA	1:B:223:LEU:O	1.99	0.63
1:B:223:LEU:C	1:B:223:LEU:HD23	2.20	0.63
1:A:71:LEU:HD12	1:A:186:LEU:HD11	1.79	0.63
1:B:103:LYS:O	1:B:106:LYS:HG3	1.99	0.63
1:A:51:HIS:CD2	2:A:1001:YSA:H5'2	2.33	0.62
1:A:148:VAL:O	1:A:152:ILE:HG12	1.99	0.62
1:B:113:ASP:OD1	1:B:116:CYS:HB3	1.99	0.62
1:B:38:CYS:HB3	1:B:58:LEU:HD11	1.80	0.61
1:B:134:ASN:ND2	1:B:136:LEU:HB2	2.15	0.61
1:B:42:PRO:HG2	1:B:101:VAL:HG22	1.81	0.61
1:A:49:LEU:HD11	1:A:260:TRP:HH2	1.66	0.61
1:A:178:LEU:HD12	1:A:178:LEU:H	1.66	0.61
1:B:235:LYS:NZ	1:B:238:LYS:HB2	2.15	0.61
1:B:132:ASN:H	1:B:132:ASN:HD22	1.49	0.61
1:A:237:GLY:O	1:A:243:ALA:HA	2.00	0.60
1:B:62:GLN:HE22	1:B:113:ASP:H	1.49	0.60
1:B:13:ARG:NH2	1:B:278:MET:O	2.33	0.60
1:B:59:LYS:O	1:B:63:GLN:HG3	2.01	0.60
1:A:51:HIS:O	1:A:54:PRO:HD2	2.03	0.59
1:B:163:ARG:HD2	1:B:166:GLN:HE21	1.66	0.59
1:B:304:ALA:O	1:B:308:THR:HB	2.02	0.59
1:A:79:ILE:HG23	1:A:171:THR:HG22	1.83	0.59
1:B:7:ILE:HG22	1:B:11:GLN:HE21	1.68	0.58
1:B:291:LYS:HD2	1:B:292:ASN:ND2	2.18	0.58
1:B:13:ARG:HD3	1:B:273:LYS:O	2.03	0.58
1:B:293:SER:O	1:B:295:LYS:N	2.37	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:ASN:HA	1:A:158:LYS:HD3	1.86	0.58
1:A:254:TYR:HA	1:A:320:ALA:HA	1.86	0.57
1:B:37:VAL:HG22	1:B:38:CYS:N	2.19	0.57
1:A:78:LEU:C	1:A:79:ILE:HD12	2.25	0.57
1:B:312:HIS:HB3	1:B:316:GLY:HA3	1.84	0.57
1:B:90:LYS:HG2	1:B:91:LEU:N	2.18	0.57
1:B:34:ILE:HG12	1:B:66:HIS:CD2	2.40	0.57
1:A:54:PRO:HG2	2:A:1001:YSA:O4'	2.04	0.56
1:B:159:GLN:O	1:B:161:LEU:O	2.23	0.56
1:A:223:LEU:C	1:A:223:LEU:HD23	2.25	0.56
1:B:104:ILE:O	1:B:108:VAL:HG23	2.05	0.56
1:A:232:ASP:OD2	1:A:234:THR:HG23	2.06	0.56
1:A:235:LYS:O	1:A:236:PHE:HB2	2.06	0.55
1:A:147:SER:OG	1:A:150:GLN:HG2	2.06	0.55
1:A:134:ASN:HD21	1:A:136:LEU:CB	2.13	0.55
1:B:147:SER:HB3	1:B:150:GLN:HG2	1.88	0.55
1:A:163:ARG:HB3	1:A:166:GLN:H	1.72	0.55
1:A:102:ASP:HA	1:A:105:ARG:CD	2.34	0.55
1:B:5:ASN:O	1:B:9:GLN:HG3	2.07	0.55
1:B:179:GLN:NE2	1:B:204:ASN:HB3	2.23	0.54
1:A:132:ASN:HD22	1:A:132:ASN:C	2.10	0.54
1:A:52:LEU:HG	1:A:56:LEU:HD22	1.90	0.54
1:A:19:VAL:CG1	1:A:22:GLU:HB2	2.37	0.54
1:B:195:CYS:SG	1:B:205:ILE:HD12	2.47	0.54
1:A:8:LYS:NZ	1:A:8:LYS:HB3	2.22	0.54
1:A:100:TRP:O	1:A:104:ILE:HG12	2.08	0.53
1:A:7:ILE:O	1:A:11:GLN:HG3	2.08	0.53
1:B:202:TRP:O	1:B:205:ILE:N	2.42	0.53
1:A:144:LYS:HE3	1:B:91:LEU:HG	1.91	0.53
1:A:166:GLN:HG2	3:A:1045:HOH:O	2.08	0.53
1:B:190:TYR:HB2	1:B:192:VAL:HG23	1.92	0.52
1:A:214:ARG:HH11	1:A:214:ARG:HG3	1.75	0.52
1:B:42:PRO:CG	1:B:101:VAL:HG22	2.39	0.52
1:A:179:GLN:HG3	2:A:1001:YSA:CZ	2.39	0.52
1:B:269:TYR:CE1	1:B:287:GLU:HA	2.45	0.52
1:A:162:ASN:O	1:A:163:ARG:HG3	2.08	0.52
1:B:90:LYS:HG2	1:B:91:LEU:H	1.75	0.52
1:B:183:PHE:CZ	1:B:220:VAL:HG13	2.45	0.52
1:A:71:LEU:CD1	1:A:186:LEU:HD11	2.40	0.51
1:A:163:ARG:HH11	1:A:163:ARG:HG3	1.75	0.51
1:A:293:SER:HA	3:A:1058:HOH:O	2.11	0.51
1:A:235:LYS:CG	1:A:236:PHE:H	2.19	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:LEU:O	1:A:215:LEU:HD23	2.10	0.50
1:A:279:SER:O	1:A:281:GLU:N	2.44	0.50
1:A:104:ILE:O	1:A:108:VAL:HG23	2.11	0.50
1:B:59:LYS:HD2	1:B:111:PHE:O	2.11	0.50
1:A:279:SER:OG	1:A:282:GLU:HG2	2.12	0.50
1:A:272:LEU:CD1	1:A:286:LEU:HD23	2.41	0.50
1:B:109:ALA:HB3	1:B:110:PRO:HD3	1.93	0.50
1:B:161:LEU:O	1:B:163:ARG:N	2.44	0.50
1:B:211:LEU:HD12	1:B:215:LEU:HD23	1.93	0.50
1:A:53:VAL:HB	1:A:54:PRO:CD	2.39	0.50
1:A:279:SER:C	1:A:281:GLU:N	2.65	0.50
1:B:163:ARG:HD2	1:B:166:GLN:NE2	2.28	0.49
1:B:57:CYS:HA	1:B:60:ARG:HD2	1.94	0.49
1:A:134:ASN:HD22	1:A:137:THR:H	1.61	0.49
1:A:49:LEU:HD12	1:A:236:PHE:CE2	2.48	0.49
1:A:50:GLY:O	1:A:53:VAL:HG23	2.13	0.49
1:A:5:ASN:O	1:A:9:GLN:HG3	2.12	0.49
1:B:37:VAL:HG23	1:B:69:VAL:O	2.13	0.49
1:A:41:ASP:OD2	1:A:73:GLY:HA3	2.13	0.49
1:A:223:LEU:O	1:A:223:LEU:HD23	2.12	0.49
1:B:100:TRP:O	1:B:103:LYS:HB2	2.13	0.49
1:B:145:HIS:CD2	1:B:215:LEU:HD21	2.48	0.49
1:B:228:ILE:HD12	1:B:274:PHE:CE1	2.47	0.49
1:A:288:GLU:OE2	1:A:291:LYS:HD3	2.13	0.49
1:B:13:ARG:NH1	1:B:273:LYS:O	2.46	0.48
1:B:235:LYS:CE	1:B:238:LYS:HE3	2.43	0.48
1:B:132:ASN:HD22	1:B:132:ASN:N	2.09	0.48
1:A:52:LEU:O	1:A:56:LEU:HB2	2.13	0.48
1:A:161:LEU:O	1:B:149:ASN:OD1	2.31	0.48
1:B:96:THR:O	1:B:99:GLU:HB3	2.14	0.48
1:A:245:TRP:CD1	1:A:250:LYS:HE2	2.49	0.48
1:A:269:TYR:CZ	1:A:287:GLU:HA	2.49	0.48
1:B:34:ILE:H	1:B:66:HIS:HD2	1.62	0.48
1:A:279:SER:O	1:A:280:ILE:C	2.52	0.48
1:A:269:TYR:CE1	1:A:287:GLU:HA	2.48	0.48
1:B:114:PHE:O	1:B:115:ASP:HB2	2.12	0.48
1:B:81:ASP:HB2	1:B:175:TYR:CZ	2.49	0.48
1:A:175:TYR:OH	2:A:1001:YSA:N	2.43	0.47
1:B:13:ARG:CB	1:B:273:LYS:HB3	2.40	0.47
1:B:235:LYS:HZ1	1:B:238:LYS:HE3	1.79	0.47
1:B:56:LEU:O	1:B:60:ARG:HG3	2.15	0.47
1:B:52:LEU:HD23	1:B:275:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:ASP:HB2	1:A:175:TYR:CZ	2.49	0.47
1:B:15:LEU:O	1:B:225:VAL:HA	2.14	0.47
1:B:147:SER:O	1:B:150:GLN:HG2	2.15	0.47
1:B:201:GLN:O	1:B:205:ILE:HG12	2.14	0.47
1:A:267:ASP:O	1:A:269:TYR:N	2.47	0.47
1:A:199:SER:HB3	1:A:227:LEU:CD1	2.40	0.47
1:B:134:ASN:ND2	1:B:136:LEU:H	2.13	0.47
1:A:117:GLY:O	1:A:118:GLU:C	2.53	0.47
1:A:256:PHE:O	1:A:259:PHE:HB3	2.14	0.47
1:A:273:LYS:NZ	1:A:280:ILE:HD11	2.29	0.47
1:B:218:ASN:HD22	1:B:218:ASN:N	2.13	0.47
1:B:37:VAL:CG2	1:B:38:CYS:N	2.77	0.46
1:A:79:ILE:N	1:A:79:ILE:HD12	2.30	0.46
1:A:181:TYR:HA	1:A:211:LEU:HD23	1.97	0.46
1:B:51:HIS:O	1:B:54:PRO:HD2	2.15	0.46
2:A:1001:YSA:H5'1	2:A:1001:YSA:H8	1.97	0.46
1:B:98:GLN:HG3	3:B:1009:HOH:O	2.16	0.46
1:A:95:GLU:CD	1:A:95:GLU:H	2.17	0.46
1:B:54:PRO:HG2	2:B:1002:YSA:C1'	2.46	0.46
1:A:37:VAL:HG12	1:A:38:CYS:N	2.31	0.46
1:A:49:LEU:HD21	1:A:260:TRP:CZ2	2.51	0.46
1:B:257:TYR:CZ	1:B:321:LYS:HE3	2.51	0.46
1:B:235:LYS:HZ2	1:B:238:LYS:HB2	1.80	0.45
1:A:291:LYS:HG2	1:A:292:ASN:ND2	2.31	0.45
1:B:41:ASP:OD2	1:B:73:GLY:HA3	2.17	0.45
1:A:166:GLN:HG3	1:A:167:GLY:N	2.31	0.45
1:A:237:GLY:O	1:A:244:VAL:HG23	2.16	0.45
1:A:135:VAL:HG13	1:A:136:LEU:N	2.32	0.45
1:A:111:PHE:O	1:A:112:LEU:HD23	2.16	0.45
1:A:209:ILE:HA	1:A:220:VAL:CG1	2.47	0.45
1:B:165:ASP:N	1:B:165:ASP:OD2	2.50	0.45
1:A:20:THR:HG23	1:A:222:GLY:O	2.17	0.45
2:B:1002:YSA:H5'1	2:B:1002:YSA:H8	1.98	0.44
1:B:34:ILE:HG12	1:B:66:HIS:HD2	1.81	0.44
1:B:18:GLN:HB2	1:B:202:TRP:CZ3	2.52	0.44
1:A:53:VAL:CG2	1:A:228:ILE:HD12	2.47	0.44
1:B:248:PRO:HG3	1:B:312:HIS:ND1	2.32	0.44
1:B:245:TRP:CD1	1:B:250:LYS:HB3	2.52	0.44
1:B:132:ASN:H	1:B:132:ASN:ND2	2.13	0.44
1:A:25:LEU:HB2	1:A:221:PHE:CD2	2.52	0.44
1:B:54:PRO:HG2	2:B:1002:YSA:O4'	2.16	0.44
1:A:41:ASP:HA	1:A:42:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:ILE:HG21	1:B:222:GLY:HA3	1.99	0.44
1:B:37:VAL:HB	1:B:69:VAL:HB	2.00	0.44
1:A:102:ASP:HA	1:A:105:ARG:CG	2.48	0.44
1:B:218:ASN:ND2	1:B:218:ASN:N	2.65	0.43
1:A:236:PHE:C	1:A:238:LYS:H	2.21	0.43
1:A:248:PRO:HG3	1:A:312:HIS:ND1	2.33	0.43
1:B:193:VAL:HA	1:B:220:VAL:HG22	1.99	0.43
1:A:286:LEU:HD21	1:A:299:ALA:HA	2.01	0.43
1:A:195:CYS:SG	3:A:1007:HOH:O	2.44	0.43
1:B:8:LYS:HD2	1:B:8:LYS:HA	1.76	0.43
1:B:217:GLN:C	1:B:218:ASN:HD22	2.22	0.43
1:A:18:GLN:HB2	1:A:202:TRP:CZ3	2.54	0.43
1:A:49:LEU:HD12	1:A:236:PHE:CZ	2.54	0.43
1:A:256:PHE:HE2	1:A:307:VAL:HG12	1.83	0.43
1:B:19:VAL:CG1	1:B:22:GLU:HB2	2.48	0.43
1:A:79:ILE:HD11	1:B:136:LEU:HD22	2.01	0.43
1:A:237:GLY:O	1:A:244:VAL:N	2.52	0.43
1:A:260:TRP:CZ2	1:A:307:VAL:HG11	2.55	0.42
1:B:75:ALA:HB2	1:B:127:TYR:HA	2.00	0.42
1:A:132:ASN:ND2	1:A:132:ASN:C	2.73	0.42
1:B:72:VAL:HG11	1:B:101:VAL:HG13	2.00	0.42
1:A:268:VAL:HG13	1:A:269:TYR:N	2.34	0.42
1:B:41:ASP:HA	1:B:42:PRO:HD3	1.83	0.42
1:B:76:THR:HB	1:B:175:TYR:OH	2.19	0.42
1:B:75:ALA:O	1:B:78:LEU:HB2	2.19	0.42
1:B:78:LEU:HA	1:B:78:LEU:HD12	1.90	0.42
1:B:181:TYR:HA	1:B:211:LEU:HD23	2.01	0.42
1:A:138:PHE:CG	1:B:135:VAL:HG21	2.55	0.42
1:B:293:SER:OG	1:B:295:LYS:HD3	2.20	0.42
1:A:145:HIS:ND1	1:A:214:ARG:NH1	2.68	0.42
1:A:177:LEU:N	1:A:177:LEU:HD12	2.34	0.42
1:A:235:LYS:HG3	1:A:238:LYS:HB3	2.02	0.41
1:B:311:VAL:HG12	1:B:312:HIS:CD2	2.55	0.41
1:A:269:TYR:CE2	1:A:287:GLU:HG3	2.55	0.41
1:B:216:HIS:O	1:B:217:GLN:HB2	2.20	0.41
1:A:42:PRO:HD2	1:A:77:GLY:HA3	2.01	0.41
1:A:95:GLU:CD	1:A:95:GLU:N	2.73	0.41
1:A:13:ARG:NH2	1:A:276:THR:O	2.53	0.41
1:B:293:SER:C	1:B:295:LYS:H	2.23	0.41
1:B:140:ARG:O	1:B:144:LYS:HB2	2.20	0.41
1:B:263:THR:HG22	1:B:264:ALA:O	2.21	0.41
1:B:161:LEU:C	1:B:163:ARG:N	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:LYS:CG	1:A:236:PHE:N	2.66	0.41
1:B:34:ILE:H	1:B:66:HIS:CD2	2.38	0.41
1:A:273:LYS:HZ2	1:A:280:ILE:HD11	1.85	0.41
1:B:284:ASN:HA	1:B:284:ASN:HD22	1.63	0.41
1:B:20:THR:HG21	1:B:209:ILE:HD13	2.02	0.41
1:B:221:PHE:CD1	1:B:221:PHE:N	2.88	0.41
1:B:206:THR:O	1:B:209:ILE:N	2.54	0.41
1:A:235:LYS:HB3	1:A:235:LYS:NZ	2.35	0.41
1:A:174:SER:O	1:A:175:TYR:C	2.59	0.40
1:A:209:ILE:HA	1:A:220:VAL:HG12	2.02	0.40
1:A:152:ILE:HG23	1:A:161:LEU:HD13	2.03	0.40
1:A:195:CYS:SG	1:A:205:ILE:CD1	3.07	0.40
1:B:245:TRP:HB2	1:B:250:LYS:HB2	2.03	0.40
1:B:177:LEU:N	1:B:177:LEU:HD12	2.37	0.40
1:B:280:ILE:HD12	1:B:280:ILE:HA	1.96	0.40
1:B:36:LEU:HD13	1:B:194:LEU:HD23	2.03	0.40
1:A:183:PHE:CE1	1:A:220:VAL:HG21	2.56	0.40
1:B:85:LYS:HE3	1:B:89:ARG:NE	2.37	0.40
1:B:238:LYS:HG3	1:B:239:THR:N	2.37	0.40
1:A:76:THR:HB	1:A:175:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

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	316/318 (99%)	277 (88%)	32 (10%)	7 (2%)	10	25
1	B	316/318 (99%)	279 (88%)	30 (10%)	7 (2%)	10	25
All	All	632/636 (99%)	556 (88%)	62 (10%)	14 (2%)	10	25

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	CYS
1	A	268	VAL
1	B	115	ASP
1	A	118	GLU
1	A	236	PHE
1	B	159	GLN
1	B	162	ASN
1	B	234	THR
1	B	243	ALA
1	B	294	GLY
1	A	163	ARG
1	A	233	GLY
1	B	202	TRP
1	A	280	ILE

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	264/264 (100%)	243 (92%)	21 (8%)	17	37
1	B	264/264 (100%)	244 (92%)	20 (8%)	19	41
All	All	528/528 (100%)	487 (92%)	41 (8%)	18	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	55	LEU
1	A	56	LEU
1	A	57	CYS
1	A	76	THR
1	A	78	LEU
1	A	89	ARG
1	A	102	ASP
1	A	105	ARG
1	A	113	ASP
1	A	116	CYS
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	147	SER
1	A	160	ARG
1	A	183	PHE
1	A	214	ARG
1	A	217	GLN
1	A	220	VAL
1	A	235	LYS
1	A	301	TYR
1	A	318	GLN
1	B	43	THR
1	B	55	LEU
1	B	76	THR
1	B	78	LEU
1	B	85	LYS
1	B	106	LYS
1	B	132	ASN
1	B	155	GLU
1	B	159	GLN
1	B	183	PHE
1	B	199	SER
1	B	220	VAL
1	B	221	PHE
1	B	232	ASP
1	B	261	ILE
1	B	286	LEU
1	B	292	ASN
1	B	295	LYS
1	B	305	GLU
1	B	308	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	134	ASN
1	A	166	GLN
1	A	176	ASN
1	A	179	GLN
1	A	204	ASN
1	A	217	GLN
1	A	218	ASN
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	292	ASN
1	B	9	GLN
1	B	11	GLN
1	B	62	GLN
1	B	66	HIS
1	B	132	ASN
1	B	134	ASN
1	B	149	ASN
1	B	150	GLN
1	B	159	GLN
1	B	166	GLN
1	B	218	ASN
1	B	219	GLN
1	B	262	ASN
1	B	284	ASN
1	B	292	ASN
1	B	306	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	YSA	A	1001	-	38,38,38	2.57	8 (21%)	56,56,56	2.34	7 (12%)
2	YSA	B	1002	-	38,38,38	2.55	7 (18%)	56,56,56	2.34	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YSA	A	1001	-	-	1/23/39/39	0/2/4/4
2	YSA	B	1002	-	-	1/23/39/39	0/2/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	YSA	OAE-SBI	8.95	1.50	1.42
2	A	1001	YSA	OAD-SBI	8.95	1.50	1.42
2	B	1002	YSA	OAE-SBI	8.89	1.50	1.42
2	B	1002	YSA	OAD-SBI	8.87	1.50	1.42
2	A	1001	YSA	O5'-SBI	-7.12	1.50	1.58
2	B	1002	YSA	O5'-SBI	-7.00	1.50	1.58
2	B	1002	YSA	SBI-NAT	3.11	1.63	1.60
2	A	1001	YSA	C4-N9	-2.97	1.33	1.37
2	A	1001	YSA	SBI-NAT	2.96	1.63	1.60
2	B	1002	YSA	C4-N9	-2.87	1.33	1.37
2	A	1001	YSA	C-NAT	-2.42	1.33	1.37
2	B	1002	YSA	C-NAT	-2.34	1.33	1.37
2	B	1002	YSA	O4'-C1'	2.03	1.44	1.41
2	A	1001	YSA	O4'-C1'	2.02	1.44	1.41
2	A	1001	YSA	C8-N9	-2.01	1.33	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	YSA	OAE-SBI-OAD	-11.11	109.87	121.45
2	A	1001	YSA	OAE-SBI-OAD	-10.81	110.18	121.45
2	B	1002	YSA	N3-C2-N1	-9.29	120.94	128.71
2	A	1001	YSA	N3-C2-N1	-8.93	121.24	128.71
2	A	1001	YSA	O4'-C1'-N9	5.84	113.88	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	YSA	N3-C4-N9	4.53	133.61	125.43
2	A	1001	YSA	N3-C4-N9	4.37	133.33	125.43
2	B	1002	YSA	O4'-C1'-N9	4.04	112.19	108.44
2	B	1002	YSA	C5-C4-N3	-2.87	119.45	125.70
2	A	1001	YSA	C5-C4-N3	-2.79	119.64	125.70
2	B	1002	YSA	C2-N3-C4	2.49	121.10	114.01
2	B	1002	YSA	O5'-C5'-C4'	2.45	112.46	107.81
2	A	1001	YSA	C2-N3-C4	2.42	120.89	114.01
2	B	1002	YSA	C4-C5-N7	-2.33	107.52	109.52
2	A	1001	YSA	C4-C5-N7	-2.17	107.66	109.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1002	YSA	O5'-SBI-NAT-C
2	A	1001	YSA	O5'-SBI-NAT-C

There are no ring outliers.

5.7 Other polymers ⓘ

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 ⓘ

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	318/318 (100%)	-0.45	2 (0%) 86 90	17, 39, 69, 111	0
1	B	318/318 (100%)	-0.51	0 100 100	21, 37, 66, 103	0
All	All	636/636 (100%)	-0.48	2 (0%) 91 95	17, 39, 67, 111	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LYS	2.2
1	A	237	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	YSA	B	1002	35/35	0.15	0.66	23,35,46,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	YSA	A	1001	35/35	0.13	0.24	24,37,46,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.