



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WLE  
Title : Crystal Structure of mammalian mitochondrial seryl-tRNA synthetase complexed with seryl-adenylate  
Authors : Chimnaronk, S.; Jeppesen, M.G.; Suzuki, T.; Nyborg, J.; Watanabe, K.  
Deposited on : 2004-06-25  
Resolution : 1.65 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

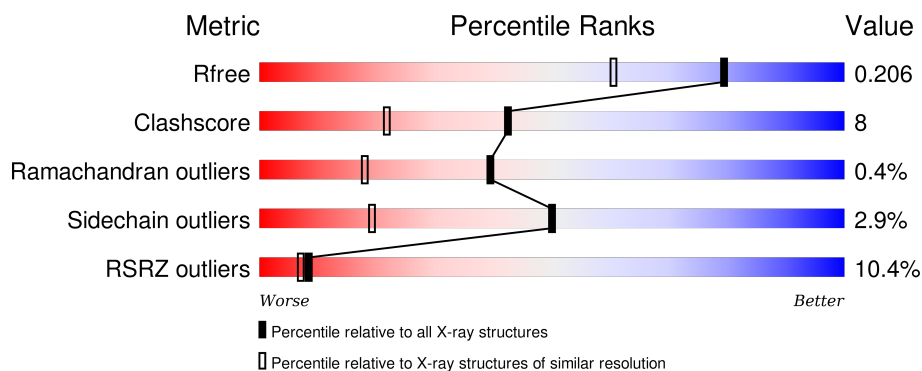
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	501	
1	B	501	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8106 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	465	Total	C	N	O	S	0	0	0
			3701	2337	661	687	16			
1	B	469	Total	C	N	O	S	0	0	0
			3736	2357	667	696	16			

There are 34 discrepancies between the modelled and reference sequences:

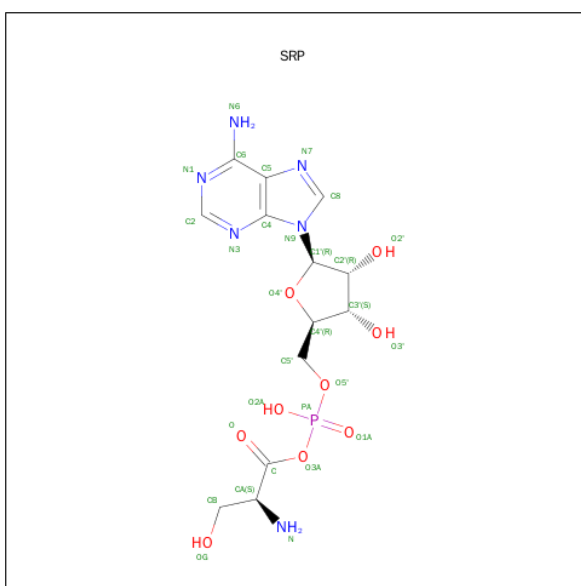
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9N0F3
A	2	GLY	-	EXPRESSION TAG	UNP Q9N0F3
A	3	HIS	-	EXPRESSION TAG	UNP Q9N0F3
A	4	HIS	-	EXPRESSION TAG	UNP Q9N0F3
A	5	HIS	-	EXPRESSION TAG	UNP Q9N0F3
A	6	HIS	-	EXPRESSION TAG	UNP Q9N0F3
A	7	HIS	-	EXPRESSION TAG	UNP Q9N0F3
A	8	HIS	-	EXPRESSION TAG	UNP Q9N0F3
A	9	SER	-	EXPRESSION TAG	UNP Q9N0F3
A	10	SER	-	EXPRESSION TAG	UNP Q9N0F3
A	11	GLY	-	EXPRESSION TAG	UNP Q9N0F3
A	12	LEU	-	EXPRESSION TAG	UNP Q9N0F3
A	13	VAL	-	EXPRESSION TAG	UNP Q9N0F3
A	14	PRO	-	EXPRESSION TAG	UNP Q9N0F3
A	15	ARG	-	EXPRESSION TAG	UNP Q9N0F3
A	16	GLY	-	EXPRESSION TAG	UNP Q9N0F3
A	17	SER	-	EXPRESSION TAG	UNP Q9N0F3
B	1	MET	-	EXPRESSION TAG	UNP Q9N0F3
B	2	GLY	-	EXPRESSION TAG	UNP Q9N0F3
B	3	HIS	-	EXPRESSION TAG	UNP Q9N0F3
B	4	HIS	-	EXPRESSION TAG	UNP Q9N0F3
B	5	HIS	-	EXPRESSION TAG	UNP Q9N0F3
B	6	HIS	-	EXPRESSION TAG	UNP Q9N0F3
B	7	HIS	-	EXPRESSION TAG	UNP Q9N0F3
B	8	HIS	-	EXPRESSION TAG	UNP Q9N0F3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	SER	-	EXPRESSION TAG	UNP Q9N0F3
B	10	SER	-	EXPRESSION TAG	UNP Q9N0F3
B	11	GLY	-	EXPRESSION TAG	UNP Q9N0F3
B	12	LEU	-	EXPRESSION TAG	UNP Q9N0F3
B	13	VAL	-	EXPRESSION TAG	UNP Q9N0F3
B	14	PRO	-	EXPRESSION TAG	UNP Q9N0F3
B	15	ARG	-	EXPRESSION TAG	UNP Q9N0F3
B	16	GLY	-	EXPRESSION TAG	UNP Q9N0F3
B	17	SER	-	EXPRESSION TAG	UNP Q9N0F3

- Molecule 2 is SERYL ADENYLATE (three-letter code: SRP) (formula:  $C_{13}H_{19}N_6O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	13	6	9	1		
2	B	1	Total	C	N	O	P	0	0
			29	13	6	9	1		

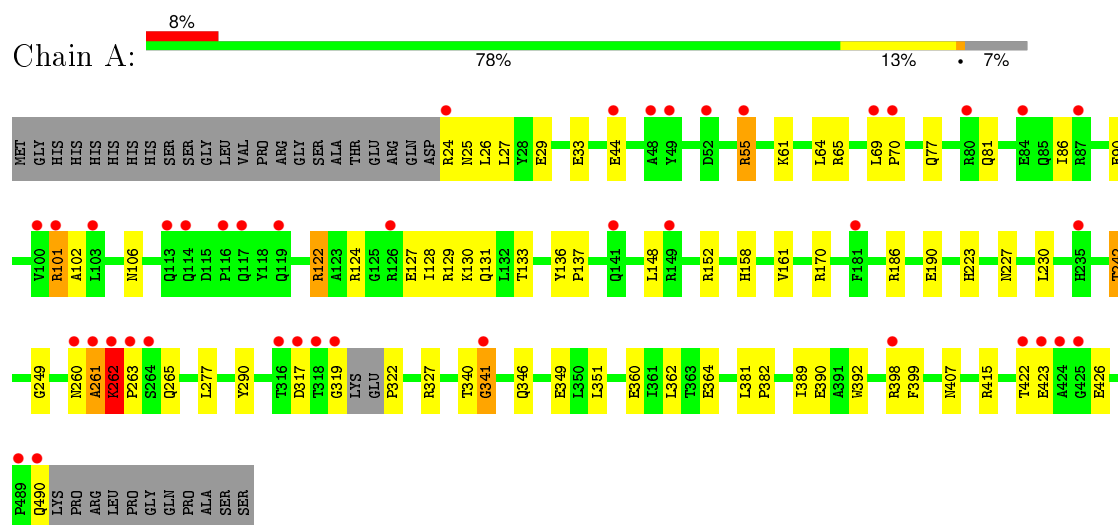
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total	O	0	0
			260	260		
3	B	351	Total	O	0	0
			351	351		

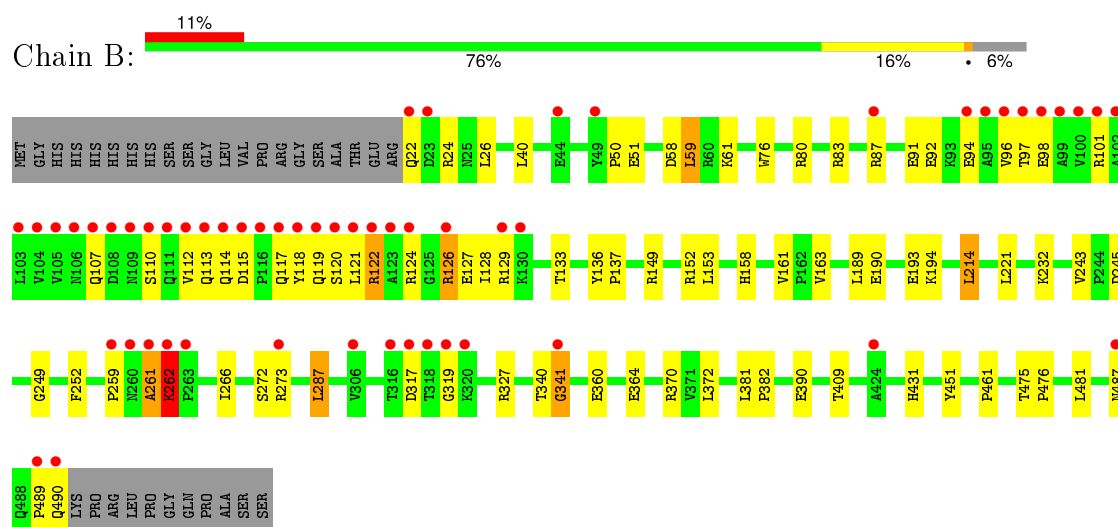
### 3 Residue-property plots [i](#)

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: Seryl-tRNA synthetase



#### • Molecule 1: Seryl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.86Å 230.35Å 135.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65 42.07 – 1.64	Depositor EDS
% Data completeness (in resolution range)	96.2 (10.00-1.65) 96.1 (42.07-1.64)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.64Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210 , 0.226 0.212 , 0.206	Depositor DCC
$R_{free}$ test set	14352 reflections (9.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 145388 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.29	0/3783	0.57	1/5127 (0.0%)
1	B	0.31	0/3819	0.65	4/5177 (0.1%)
All	All	0.30	0/7602	0.61	5/10304 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	LYS	C-N-CD	10.94	151.38	128.40
1	B	261	ALA	N-CA-C	-7.02	92.05	111.00
1	B	262	LYS	C-N-CA	-6.71	93.83	122.00
1	A	261	ALA	N-CA-C	-5.51	96.11	111.00
1	B	262	LYS	CB-CA-C	5.51	121.42	110.40

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	3701	0	3670	66	0
1	B	3736	0	3701	64	0
2	A	29	0	18	0	0
2	B	29	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	260	0	0	4	0
3	B	351	0	0	4	0
All	All	8106	0	7407	124	0

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 8.

All (124) 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:130:LYS:O	1:A:133:THR:HG22	1.67	0.94
1:A:101:ARG:HH21	1:A:101:ARG:HB3	1.40	0.87
1:A:122:ARG:HB3	1:A:122:ARG:HH21	1.46	0.79
1:B:370:ARG:HD2	1:B:390:GLU:OE1	1.83	0.78
1:B:118:TYR:O	1:B:122:ARG:HB3	1.87	0.74
1:B:261:ALA:C	1:B:262:LYS:HD3	2.08	0.73
1:A:101:ARG:NH2	1:A:101:ARG:HB3	2.02	0.73
1:A:242:THR:HB	1:B:214:LEU:HB2	1.73	0.69
1:A:262:LYS:HD2	1:A:262:LYS:C	2.13	0.68
1:A:422:THR:OG1	1:A:426:GLU:HG2	1.94	0.68
1:B:58:ASP:O	1:B:61:LYS:HD2	1.96	0.66
1:B:94:GLU:O	1:B:98:GLU:HG2	1.95	0.66
1:A:55:ARG:HD3	1:A:55:ARG:O	1.96	0.65
1:A:319:GLY:HA2	1:A:327:ARG:HD2	1.80	0.64
1:A:186:ARG:HD3	1:A:190:GLU:OE2	1.97	0.63
1:A:61:LYS:NZ	1:A:61:LYS:HB3	2.14	0.63
1:B:262:LYS:N	1:B:262:LYS:HD3	2.14	0.62
1:B:243:VAL:HG11	1:B:287:LEU:HD13	1.81	0.62
1:A:262:LYS:HB3	1:A:263:PRO:CD	2.30	0.62
1:B:340:THR:OG1	1:B:341:GLY:N	2.32	0.61
1:B:120:SER:C	1:B:121:LEU:HD22	2.20	0.61
1:B:129:ARG:O	1:B:133:THR:HG23	2.00	0.60
1:B:26:LEU:HD13	1:B:249:GLY:HA3	1.84	0.60
1:A:263:PRO:HG2	3:A:1150:HOH:O	2.03	0.59
1:B:136:TYR:HB2	1:B:137:PRO:HD3	1.84	0.59
1:A:340:THR:OG1	1:A:341:GLY:N	2.35	0.59
1:A:262:LYS:HB3	1:A:263:PRO:HD3	1.84	0.59
1:B:149:ARG:HH11	1:B:152:ARG:CZ	2.17	0.58
1:A:136:TYR:HB2	1:A:137:PRO:HD3	1.85	0.58
1:B:232:LYS:HE2	3:B:1238:HOH:O	2.03	0.58
1:A:122:ARG:CB	1:A:122:ARG:HH21	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLN:O	1:B:112:VAL:HG23	2.04	0.56
1:B:259:PRO:HA	1:B:266:ILE:HD12	1.87	0.56
1:B:117:GLN:OE1	1:B:121:LEU:HG	2.06	0.56
1:B:252:PHE:HB2	1:B:259:PRO:HG3	1.87	0.56
1:B:489:PRO:O	1:B:490:GLN:HG3	2.06	0.55
1:B:119:GLN:O	1:B:120:SER:HB2	2.07	0.54
1:B:94:GLU:O	1:B:97:THR:HG22	2.09	0.53
1:B:124:ARG:HD3	1:B:124:ARG:O	2.08	0.53
1:A:102:ALA:O	1:A:106:ASN:HB2	2.08	0.53
1:B:190:GLU:HG2	1:B:194:LYS:HE2	1.91	0.53
1:A:341:GLY:HA3	1:A:346:GLN:HG2	1.91	0.53
1:A:170:ARG:HD2	3:A:1076:HOH:O	2.08	0.53
1:B:149:ARG:HE	1:B:152:ARG:NH1	2.07	0.53
1:B:122:ARG:C	1:B:122:ARG:HD3	2.29	0.52
1:A:381:LEU:H	1:A:382:PRO:HD2	1.74	0.52
1:B:262:LYS:CD	1:B:262:LYS:N	2.73	0.52
1:A:101:ARG:HD2	1:A:101:ARG:C	2.29	0.52
1:B:272:SER:C	1:B:273:ARG:HD2	2.30	0.51
1:A:24:ARG:HD3	1:A:29:GLU:OE1	2.11	0.51
1:A:265:GLN:HB3	3:A:1037:HOH:O	2.11	0.51
1:A:290:TYR:CE2	1:B:481:LEU:HD11	2.46	0.51
1:A:86:ILE:O	1:A:90:GLU:HG3	2.11	0.50
1:B:26:LEU:HD12	1:B:259:PRO:HG2	1.92	0.50
1:B:381:LEU:H	1:B:382:PRO:HD2	1.76	0.50
1:B:149:ARG:HE	1:B:152:ARG:HH11	1.59	0.50
1:B:80:ARG:NH2	1:B:83:ARG:HH21	2.10	0.50
1:A:64:LEU:N	1:A:64:LEU:HD22	2.27	0.50
1:A:346:GLN:O	1:A:349:GLU:HG2	2.12	0.49
1:A:223:HIS:CE1	1:A:227:ASN:HD21	2.30	0.49
1:A:124:ARG:O	1:A:128:ILE:HG13	2.12	0.49
1:B:360:GLU:O	1:B:364:GLU:HG3	2.11	0.49
1:B:92:GLU:O	1:B:96:VAL:HG23	2.13	0.49
1:A:360:GLU:O	1:A:364:GLU:HG3	2.12	0.49
1:A:262:LYS:HE2	1:A:263:PRO:HD3	1.94	0.48
1:A:158:HIS:HB3	1:A:161:VAL:HG23	1.95	0.48
1:A:242:THR:CG2	1:B:214:LEU:HB2	2.44	0.48
1:A:381:LEU:N	1:A:382:PRO:HD2	2.29	0.48
1:B:124:ARG:O	1:B:128:ILE:HG13	2.13	0.47
1:A:262:LYS:HD2	1:A:263:PRO:N	2.28	0.47
1:A:262:LYS:CE	1:A:263:PRO:HD3	2.45	0.47
1:B:451:TYR:CE2	1:B:461:PRO:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TRP:O	1:B:80:ARG:HG2	2.15	0.47
1:A:129:ARG:HG3	1:A:129:ARG:HH21	1.79	0.47
1:A:322:PRO:HG2	3:A:1064:HOH:O	2.13	0.46
1:A:26:LEU:HG	1:A:260:ASN:HD21	1.80	0.46
1:B:94:GLU:C	1:B:97:THR:HG22	2.35	0.46
1:A:242:THR:CB	1:B:214:LEU:HB2	2.43	0.45
1:A:55:ARG:C	1:A:55:ARG:HD3	2.37	0.45
1:A:44:GLU:HA	1:A:44:GLU:OE1	2.16	0.45
1:A:242:THR:HG21	3:B:1002:HOH:O	2.16	0.45
1:A:242:THR:HG22	3:B:1007:HOH:O	2.17	0.45
1:B:87:ARG:O	1:B:91:GLU:HG3	2.17	0.45
1:A:64:LEU:O	1:A:65:ARG:HD3	2.17	0.44
1:B:319:GLY:HA3	1:B:327:ARG:NH2	2.32	0.44
1:A:242:THR:CG2	3:B:1007:HOH:O	2.66	0.44
1:B:59:LEU:HG	1:B:163:VAL:HG13	2.01	0.43
1:A:415:ARG:HG3	1:A:415:ARG:HH21	1.82	0.43
1:A:77:GLN:O	1:A:81:GLN:HG3	2.18	0.43
1:B:126:ARG:HD2	1:B:127:GLU:N	2.33	0.43
1:B:126:ARG:HG2	1:B:126:ARG:HH21	1.84	0.43
1:A:351:LEU:HD22	1:A:407:ASN:HB2	1.99	0.43
1:A:362:LEU:CD1	1:A:389:ILE:HG21	2.49	0.43
1:B:101:ARG:HD3	1:B:101:ARG:C	2.38	0.43
1:A:340:THR:O	1:A:341:GLY:O	2.36	0.43
1:B:50:PRO:HG2	1:B:51:GLU:OE2	2.19	0.43
1:A:127:GLU:HG3	1:A:131:GLN:HE21	1.84	0.43
1:B:124:ARG:NH2	1:B:128:ILE:HG12	2.34	0.43
1:A:490:GLN:O	1:A:490:GLN:HG3	2.19	0.42
1:A:26:LEU:HD13	1:A:249:GLY:HA3	2.01	0.42
1:A:148:LEU:O	1:A:152:ARG:HD2	2.19	0.42
1:B:158:HIS:HB3	1:B:161:VAL:HG23	2.00	0.42
1:A:25:ASN:OD1	1:A:27:LEU:HB2	2.19	0.42
1:B:189:LEU:O	1:B:193:GLU:HG3	2.19	0.42
1:B:381:LEU:N	1:B:382:PRO:HD2	2.34	0.42
1:A:261:ALA:O	1:A:262:LYS:C	2.58	0.42
1:A:29:GLU:O	1:A:33:GLU:HG2	2.20	0.42
1:B:22:GLN:OE1	1:B:24:ARG:HG3	2.19	0.42
1:B:370:ARG:HD3	1:B:372:LEU:HD21	2.01	0.42
1:B:272:SER:O	1:B:273:ARG:HD2	2.20	0.41
1:B:59:LEU:HA	1:B:59:LEU:HD12	1.91	0.41
1:A:242:THR:HG21	1:B:214:LEU:HD22	2.01	0.41
1:A:392:TRP:CZ3	1:A:398:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HB	1:B:214:LEU:CB	2.48	0.41
1:B:98:GLU:OE2	1:B:98:GLU:HA	2.19	0.41
1:A:319:GLY:HA2	1:A:327:ARG:CD	2.49	0.41
1:A:69:LEU:HB2	1:A:70:PRO:HD3	2.03	0.41
1:B:340:THR:O	1:B:341:GLY:O	2.39	0.41
1:B:451:TYR:CZ	1:B:461:PRO:HG3	2.55	0.41
1:B:475:THR:HA	1:B:476:PRO:HD3	1.86	0.41
1:A:260:ASN:O	1:A:261:ALA:C	2.59	0.41
1:B:409:THR:O	1:B:431:HIS:HA	2.22	0.40
1:B:487:ASN:HD22	1:B:487:ASN:N	2.18	0.40
1:A:390:GLU:HB3	1:A:399:PHE:HB3	2.03	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	461/501 (92%)	448 (97%)	11 (2%)	2 (0%)	39	18
1	B	467/501 (93%)	442 (95%)	23 (5%)	2 (0%)	39	18
All	All	928/1002 (93%)	890 (96%)	34 (4%)	4 (0%)	39	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	GLY
1	B	341	GLY
1	B	110	SER
1	A	262	LYS

### 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	400/430 (93%)	391 (98%)	9 (2%)	58	30
1	B	404/430 (94%)	390 (96%)	14 (4%)	43	14
All	All	804/860 (94%)	781 (97%)	23 (3%)	50	19

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	101	ARG
1	A	122	ARG
1	A	230	LEU
1	A	242	THR
1	A	262	LYS
1	A	277	LEU
1	A	317	ASP
1	A	423	GLU
1	B	40	LEU
1	B	59	LEU
1	B	113	GLN
1	B	114	GLN
1	B	115	ASP
1	B	122	ARG
1	B	126	ARG
1	B	153	LEU
1	B	214	LEU
1	B	221	LEU
1	B	245	ASP
1	B	262	LYS
1	B	287	LEU
1	B	317	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	85	GLN
1	A	111	GLN
1	A	131	GLN
1	A	141	GLN
1	A	227	ASN
1	A	260	ASN
1	A	434	ASN
1	B	77	GLN
1	B	113	GLN
1	B	119	GLN
1	B	223	HIS
1	B	377	GLN
1	B	482	GLN
1	B	487	ASN
1	B	490	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	SRP	A	900	-	24,31,31	2.04	7 (29%)	25,46,46	3.49	9 (36%)
2	SRP	B	901	-	24,31,31	2.04	7 (29%)	25,46,46	3.51	10 (40%)

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	SRP	A	900	-	-	0/15/37/37	0/3/3/3
2	SRP	B	901	-	-	0/15/37/37	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	SRP	O5'-C5'	-4.44	1.26	1.44
2	A	900	SRP	O5'-C5'	-4.43	1.26	1.44
2	B	901	SRP	PA-O5'	-2.90	1.45	1.59
2	A	900	SRP	PA-O5'	-2.77	1.46	1.59
2	A	900	SRP	C8-N7	-2.51	1.29	1.34
2	B	901	SRP	C8-N7	-2.27	1.30	1.34
2	B	901	SRP	PA-O3A	-2.27	1.56	1.60
2	A	900	SRP	PA-O2A	-2.06	1.46	1.54
2	B	901	SRP	PA-O2A	-2.02	1.46	1.54
2	A	900	SRP	PA-O1A	-2.02	1.43	1.51
2	A	900	SRP	O4'-C1'	4.25	1.46	1.41
2	B	901	SRP	O4'-C1'	4.50	1.46	1.41
2	B	901	SRP	C4-N3	4.85	1.42	1.35
2	A	900	SRP	C4-N3	5.22	1.43	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	SRP	O5'-PA-O1A	-7.05	82.24	109.62
2	B	901	SRP	O5'-PA-O1A	-6.88	82.91	109.62
2	A	900	SRP	C5'-C4'-C3'	-4.88	95.85	115.21
2	B	901	SRP	C5'-C4'-C3'	-4.49	97.40	115.21
2	B	901	SRP	N3-C2-N1	-3.77	126.01	128.89
2	B	901	SRP	O3A-PA-O5'	-3.48	93.80	102.86
2	A	900	SRP	N3-C2-N1	-3.36	126.32	128.89
2	A	900	SRP	O3A-PA-O5'	-3.17	94.60	102.86
2	B	901	SRP	O4'-C4'-C5'	-2.85	99.14	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	900	SRP	O4'-C4'-C5'	-2.80	99.30	109.32
2	B	901	SRP	C1'-N9-C4	-2.28	123.51	126.94
2	A	900	SRP	C4-C5-N7	2.80	112.06	109.48
2	B	901	SRP	C4-C5-N7	2.88	112.13	109.48
2	B	901	SRP	O3A-PA-O1A	3.24	119.05	108.38
2	A	900	SRP	O3A-PA-O1A	3.38	119.54	108.38
2	A	900	SRP	O2A-PA-O3A	4.19	117.12	104.16
2	B	901	SRP	O2A-PA-O3A	4.26	117.35	104.16
2	A	900	SRP	O5'-C5'-C4'	12.03	153.49	109.12
2	B	901	SRP	O5'-C5'-C4'	12.18	154.03	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	465/501 (92%)	0.58	41 (8%)	12 11	14, 25, 47, 62	0
1	B	469/501 (93%)	0.83	56 (11%)	6 4	12, 20, 86, 100	0
All	All	934/1002 (93%)	0.70	97 (10%)	8 7	12, 23, 55, 100	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	VAL	19.2
1	B	105	VAL	17.3
1	B	104	VAL	13.4
1	B	120	SER	13.1
1	B	100	VAL	13.0
1	B	111	GLN	11.7
1	B	121	LEU	11.0
1	B	118	TYR	10.6
1	B	102	ALA	10.5
1	B	110	SER	10.4
1	B	116	PRO	10.2
1	B	99	ALA	10.2
1	A	318	THR	8.8
1	B	109	ASN	8.3
1	B	489	PRO	8.2
1	B	115	ASP	7.7
1	B	126	ARG	7.4
1	B	317	ASP	7.4
1	B	107	GLN	7.2
1	B	119	GLN	7.1
1	A	490	GLN	7.0
1	B	103	LEU	6.9
1	A	262	LYS	6.7
1	B	261	ALA	6.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	317	ASP	6.4
1	B	113	GLN	6.1
1	A	49	TYR	6.0
1	B	97	THR	5.9
1	B	95	ALA	5.9
1	B	341	GLY	5.9
1	B	101	ARG	5.8
1	A	319	GLY	5.8
1	B	117	GLN	5.5
1	A	260	ASN	5.3
1	B	319	GLY	5.3
1	B	122	ARG	5.3
1	B	262	LYS	5.2
1	A	489	PRO	5.1
1	B	114	GLN	5.0
1	B	318	THR	4.9
1	B	260	ASN	4.9
1	B	49	TYR	4.6
1	B	129	ARG	4.5
1	A	341	GLY	4.5
1	A	263	PRO	4.4
1	A	44	GLU	4.4
1	A	261	ALA	4.4
1	B	490	GLN	4.3
1	B	108	ASP	4.3
1	A	48	ALA	4.2
1	A	55	ARG	4.0
1	B	259	PRO	3.9
1	A	424	ALA	3.8
1	B	106	ASN	3.8
1	A	423	GLU	3.7
1	B	124	ARG	3.7
1	A	69	LEU	3.6
1	B	123	ALA	3.5
1	B	98	GLU	3.5
1	B	273	ARG	3.5
1	B	87	ARG	3.4
1	A	113	GLN	3.4
1	A	87	ARG	3.3
1	B	320	LYS	3.2
1	A	103	LEU	3.2
1	A	101	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	487	ASN	3.1
1	A	316	THR	2.9
1	A	24	ARG	2.9
1	A	117	GLN	2.9
1	B	22	GLN	2.9
1	A	70	PRO	2.9
1	B	316	THR	2.9
1	B	94	GLU	2.8
1	A	149	ARG	2.7
1	A	100	VAL	2.6
1	B	130	LYS	2.6
1	B	23	ASP	2.5
1	A	84	GLU	2.4
1	A	80	ARG	2.4
1	A	116	PRO	2.4
1	A	52	ASP	2.3
1	B	96	VAL	2.3
1	B	263	PRO	2.3
1	B	424	ALA	2.3
1	A	264	SER	2.2
1	A	119	GLN	2.2
1	A	181	PHE	2.2
1	A	398	ARG	2.2
1	A	114	GLN	2.1
1	B	44	GLU	2.1
1	A	141	GLN	2.1
1	A	126	ARG	2.1
1	A	425	GLY	2.1
1	B	306	VAL	2.0
1	A	422	THR	2.0
1	A	235	HIS	2.0

## 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 [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SRP	A	900	29/29	0.93	0.12	-0.34	16,21,25,27	0
2	SRP	B	901	29/29	0.94	0.10	-0.56	14,17,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.