



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:29 am BST

PDB ID : 2ZR3  
Title : Crystal structure of seryl-tRNA synthetase from *Pyrococcus horikoshii*  
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2008-08-22  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

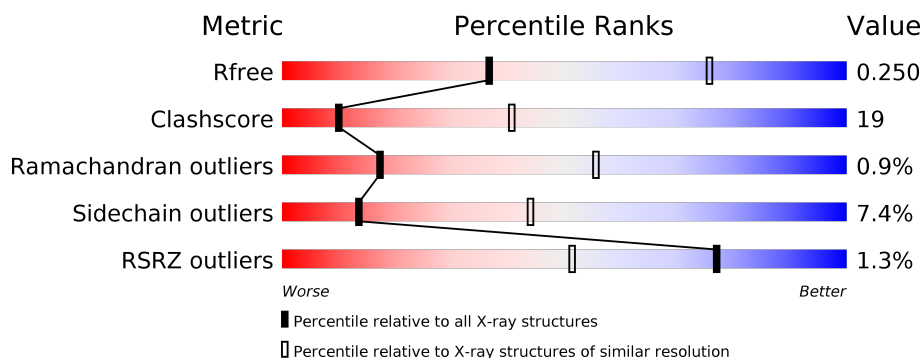
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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  $\leq 5\%$ . 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	455	 57% 38% • •
1	B	455	 2% 62% 31% 5% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7446 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	448	Total	C	N	O	S	0	0	0
			3708	2382	647	671	8			
1	B	448	Total	C	N	O	S	0	0	0
			3708	2382	647	671	8			

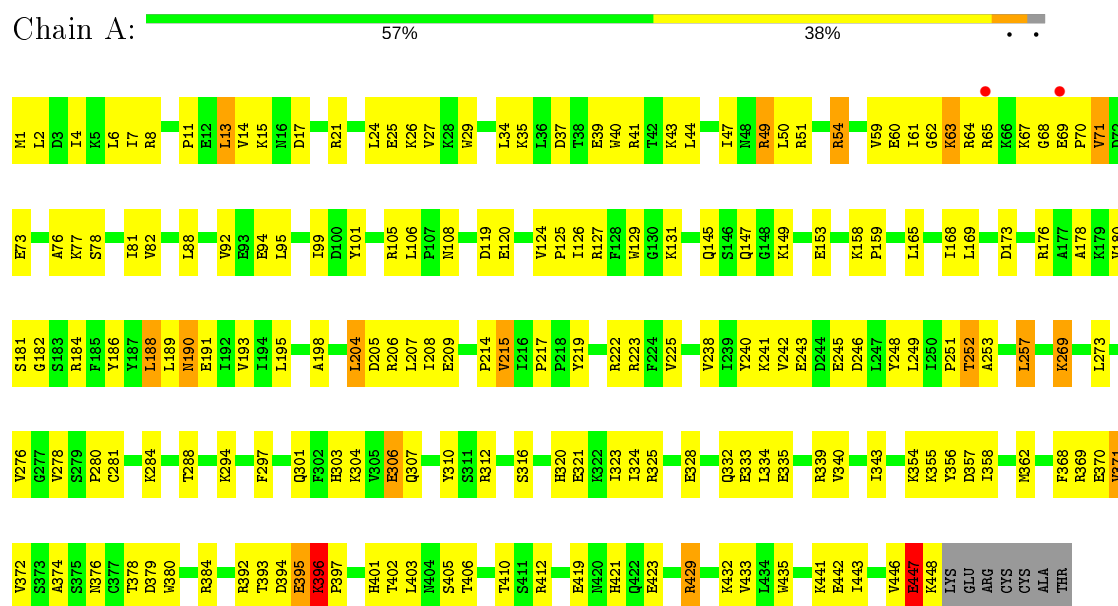
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	17	Total	O	0	0
			17	17		

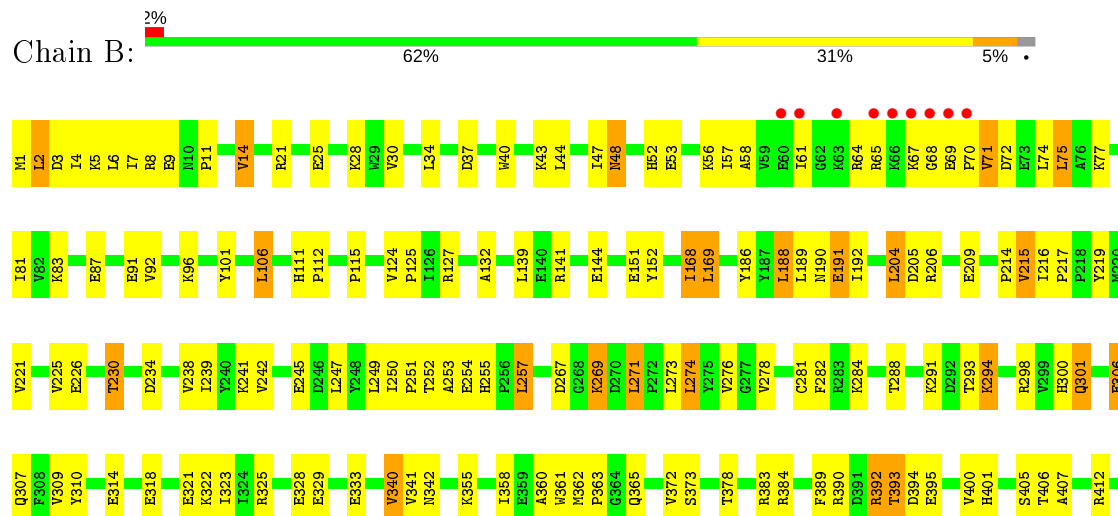
### 3 Residue-property plots

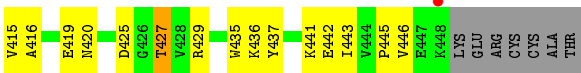
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.65Å 120.27Å 127.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 3.00 48.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.57-3.00) 99.9 (48.57-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.258 0.185 , 0.250	Depositor DCC
$R_{free}$ test set	1537 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 70.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.43	0/3792	0.70	1/5120 (0.0%)
1	B	0.45	0/3792	0.71	2/5120 (0.0%)
All	All	0.44	0/7584	0.70	3/10240 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	GLU	N-CA-C	5.08	124.72	111.00
1	A	395	GLU	N-CA-C	5.08	124.71	111.00
1	B	407	ALA	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3708	0	3750	156	0
1	B	3708	0	3750	137	0
2	A	13	0	0	1	0
2	B	17	0	0	0	0
All	All	7446	0	7500	284	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 19.

All (284) 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:288:THR:HG21	1:B:298:ARG:HD3	1.44	0.99
1:B:372:VAL:HB	1:B:406:THR:HB	1.55	0.89
1:A:127:ARG:HB3	1:A:340:VAL:HG22	1.55	0.87
1:A:269:LYS:HE2	1:A:269:LYS:HA	1.56	0.85
1:B:230:THR:HG21	1:B:234:ASP:OD2	1.77	0.85
1:B:318:GLU:O	1:B:322:LYS:HG3	1.79	0.82
1:B:358:ILE:HB	1:B:372:VAL:HG22	1.64	0.79
1:B:3:ASP:OD1	1:B:5:LYS:HE3	1.83	0.78
1:A:8:ARG:HD3	1:A:37:ASP:OD2	1.86	0.75
1:A:372:VAL:HB	1:A:406:THR:HB	1.69	0.74
1:A:446:VAL:O	1:A:447:GLU:HB2	1.85	0.74
1:B:43:LYS:HE2	1:B:91:GLU:OE2	1.88	0.74
1:B:52:HIS:NE2	1:B:56:LYS:HE3	2.02	0.74
1:A:131:LYS:HE2	1:A:153:GLU:HB2	1.69	0.73
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.53	0.72
1:B:127:ARG:NH2	1:B:328:GLU:OE2	2.22	0.72
1:B:58:ALA:O	1:B:61:ILE:HG22	1.91	0.71
1:A:392:ARG:HH21	1:A:393:THR:HG23	1.56	0.70
1:B:291:LYS:HE3	1:B:298:ARG:NH1	2.05	0.70
1:A:11:PRO:O	1:A:14:VAL:HG12	1.91	0.70
1:A:127:ARG:HB3	1:A:340:VAL:CG2	2.22	0.70
1:A:396:LYS:NZ	1:A:397:PRO:HD2	2.08	0.69
1:B:48:ASN:HD22	1:B:48:ASN:H	1.43	0.67
1:B:40:TRP:HE1	1:B:96:LYS:HE3	1.59	0.67
1:B:427:THR:HG22	1:B:445:PRO:HD3	1.75	0.67
1:B:2:LEU:HD22	1:B:106:LEU:HB3	1.76	0.66
1:A:40:TRP:HD1	1:A:92:VAL:HG13	1.60	0.66
1:B:71:VAL:O	1:B:75:LEU:HB2	1.95	0.66
1:B:378:THR:O	1:B:401:HIS:HA	1.95	0.66
1:B:65:ARG:O	1:B:65:ARG:HD3	1.96	0.65
1:A:394:ASP:OD2	1:A:395:GLU:HG2	1.96	0.65
1:B:269:LYS:H	1:B:269:LYS:HD2	1.62	0.65
1:A:371:VAL:HG12	1:A:372:VAL:HG13	1.77	0.65
1:A:61:ILE:HG23	1:A:71:VAL:HG11	1.78	0.65
1:A:447:GLU:O	1:A:448:LYS:HB2	1.96	0.65
1:A:178:ALA:HA	1:A:182:GLY:O	1.97	0.64
1:A:249:LEU:HD21	1:B:249:LEU:HD11	1.79	0.64
1:B:253:ALA:O	1:B:257:LEU:HB2	1.97	0.64
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.63	0.64
1:B:205:ASP:O	1:B:209:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG13	1:B:245:GLU:HB2	1.79	0.64
1:B:186:TYR:CD2	1:B:188:LEU:HD13	2.32	0.63
1:A:69:GLU:N	1:A:70:PRO:HD3	2.14	0.63
1:B:273:LEU:HB2	1:B:310:TYR:HB2	1.81	0.62
1:A:59:VAL:HG23	1:A:63:LYS:HE2	1.81	0.62
1:A:147:GLN:HE21	1:A:149:LYS:HD2	1.65	0.62
1:B:276:VAL:HG13	1:B:276:VAL:O	1.99	0.62
1:B:61:ILE:HG13	1:B:71:VAL:HG11	1.81	0.62
1:B:21:ARG:HH21	1:B:21:ARG:HG2	1.64	0.62
1:A:392:ARG:HE	1:A:393:THR:H	1.45	0.61
1:B:48:ASN:HD22	1:B:48:ASN:N	1.98	0.61
1:B:1:MET:O	1:B:383:ARG:HD2	2.00	0.61
1:A:378:THR:O	1:A:401:HIS:HA	2.01	0.60
1:A:78:SER:O	1:A:82:VAL:HG23	2.01	0.60
1:B:53:GLU:O	1:B:57:ILE:HG12	2.00	0.60
1:B:291:LYS:HE3	1:B:298:ARG:HH12	1.66	0.60
1:A:195:LEU:O	1:A:198:ALA:HB3	2.01	0.60
1:A:402:THR:C	1:A:403:LEU:HD12	2.22	0.60
1:B:169:LEU:HG	1:B:443:ILE:HG22	1.82	0.59
1:B:65:ARG:HD3	1:B:65:ARG:C	2.22	0.59
1:B:21:ARG:HG2	1:B:21:ARG:NH2	2.18	0.59
1:A:251:PRO:HG2	1:A:252:THR:HG22	1.84	0.59
1:B:191:GLU:HG3	1:B:443:ILE:HG23	1.84	0.59
1:B:251:PRO:HG2	1:B:252:THR:HG22	1.84	0.59
1:B:69:GLU:N	1:B:70:PRO:HD3	2.16	0.58
1:A:190:ASN:HA	1:B:214:PRO:HG2	1.83	0.58
1:A:24:LEU:O	1:A:27:VAL:HG12	2.03	0.58
1:B:87:GLU:O	1:B:91:GLU:HG3	2.03	0.58
1:A:105:ARG:CG	1:A:105:ARG:HH11	2.17	0.57
1:B:43:LYS:O	1:B:47:ILE:HG13	2.03	0.57
1:A:222:ARG:HG3	1:A:246:ASP:OD1	2.05	0.57
1:B:436:LYS:HE2	1:B:437:TYR:CE1	2.40	0.57
1:A:37:ASP:O	1:A:41:ARG:HG2	2.04	0.57
1:A:145:GLN:HG3	2:A:457:HOH:O	2.04	0.56
1:B:425:ASP:CG	1:B:427:THR:HG23	2.25	0.56
1:A:193:VAL:HG22	1:B:216:ILE:HG13	1.88	0.56
1:B:1:MET:HE1	1:B:383:ARG:HG2	1.88	0.56
1:B:115:PRO:HD3	1:B:342:ASN:ND2	2.21	0.56
1:A:392:ARG:HB3	1:A:394:ASP:OD1	2.06	0.55
1:B:7:ILE:HD12	1:B:7:ILE:N	2.21	0.55
1:A:14:VAL:HG13	1:A:15:LYS:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:HG2	1:B:190:ASN:HA	1.89	0.55
1:A:219:TYR:CE2	1:A:280:PRO:HD2	2.42	0.54
1:A:40:TRP:CD1	1:A:92:VAL:HG13	2.42	0.54
1:A:241:LYS:HD2	1:A:248:TYR:CE2	2.42	0.54
1:B:61:ILE:HG13	1:B:71:VAL:CG1	2.38	0.54
1:B:412:ARG:O	1:B:415:VAL:HG22	2.07	0.54
1:B:67:LYS:HG2	1:B:68:GLY:H	1.71	0.54
1:B:226:GLU:OE1	1:B:255:HIS:ND1	2.40	0.54
1:B:151:GLU:O	1:B:152:TYR:HB3	2.07	0.54
1:B:61:ILE:CD1	1:B:75:LEU:HD23	2.38	0.54
1:B:83:LYS:O	1:B:87:GLU:HG3	2.08	0.53
1:A:13:LEU:HD13	1:A:13:LEU:C	2.27	0.53
1:B:141:ARG:O	1:B:144:GLU:HB3	2.09	0.53
1:A:35:LYS:O	1:A:39:GLU:HG3	2.09	0.53
1:A:396:LYS:HZ2	1:A:397:PRO:HD2	1.73	0.53
1:B:127:ARG:HH21	1:B:328:GLU:CD	2.12	0.53
1:B:242:VAL:CG1	1:B:247:LEU:HB2	2.39	0.53
1:A:376:ASN:HA	1:A:403:LEU:HG	1.91	0.53
1:B:219:TYR:O	1:B:250:ILE:HG23	2.10	0.52
1:B:5:LYS:O	1:B:9:GLU:HG3	2.09	0.52
1:B:363:PRO:HG2	1:B:420:ASN:HA	1.91	0.52
1:A:165:LEU:HD23	1:A:168:ILE:HD11	1.92	0.52
1:B:204:LEU:HD21	1:B:278:VAL:HG21	1.92	0.52
1:A:205:ASP:O	1:A:209:GLU:HG3	2.10	0.51
1:A:316:SER:HB2	1:A:376:ASN:HD21	1.75	0.51
1:A:129:TRP:CH2	1:A:332:GLN:HA	2.45	0.51
1:A:321:GLU:O	1:A:325:ARG:HG2	2.10	0.51
1:A:396:LYS:HA	1:A:396:LYS:NZ	2.25	0.51
1:A:124:VAL:O	1:A:126:ILE:HG23	2.10	0.51
1:A:304:LYS:HD3	1:A:306:GLU:OE1	2.10	0.51
1:A:14:VAL:CG1	1:A:15:LYS:N	2.73	0.51
1:B:435:TRP:CE2	1:B:441:LYS:HG2	2.45	0.51
1:A:339:ARG:O	1:A:339:ARG:HG3	2.11	0.51
1:A:362:MET:HB3	1:A:419:GLU:OE1	2.11	0.51
1:A:60:GLU:HA	1:A:63:LYS:HE3	1.93	0.51
1:B:74:LEU:O	1:B:74:LEU:HD23	2.10	0.51
1:A:392:ARG:HE	1:A:393:THR:N	2.10	0.50
1:B:425:ASP:OD2	1:B:427:THR:HG23	2.11	0.50
1:A:169:LEU:HG	1:A:443:ILE:HG22	1.94	0.50
1:A:26:LYS:HE2	1:A:29:TRP:CH2	2.47	0.50
1:A:7:ILE:HG22	1:A:34:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ARG:HD3	1:B:392:ARG:O	2.11	0.50
1:B:69:GLU:HG2	1:B:71:VAL:HG22	1.93	0.50
1:A:180:VAL:HG12	1:A:181:SER:OG	2.11	0.50
1:B:4:ILE:HD11	1:B:37:ASP:OD1	2.11	0.50
1:B:14:VAL:HG22	1:B:30:VAL:HG21	1.93	0.50
1:B:186:TYR:HD2	1:B:188:LEU:HD13	1.77	0.49
1:B:416:ALA:O	1:B:420:ASN:HB2	2.11	0.49
1:B:69:GLU:C	1:B:71:VAL:H	2.15	0.49
1:B:25:GLU:OE2	1:B:28:LYS:HD2	2.13	0.49
1:A:189:LEU:HD23	1:B:215:VAL:HB	1.94	0.49
1:A:240:TYR:HA	1:A:284:LYS:HE3	1.95	0.48
1:B:281:CYS:O	1:B:301:GLN:HA	2.13	0.48
1:B:238:VAL:HG22	1:B:239:ILE:HG13	1.94	0.48
1:A:392:ARG:HA	1:A:392:ARG:NE	2.27	0.48
1:A:423:GLU:OE2	1:A:429:ARG:HD2	2.14	0.48
1:A:219:TYR:CG	1:B:301:GLN:NE2	2.82	0.48
1:B:321:GLU:O	1:B:325:ARG:HG3	2.14	0.48
1:A:223:ARG:HB2	1:A:248:TYR:CE1	2.49	0.48
1:A:276:VAL:HG13	1:A:276:VAL:O	2.14	0.48
1:A:8:ARG:HH22	1:A:40:TRP:HZ3	1.62	0.48
1:A:173:ASP:OD2	1:A:176:ARG:HD2	2.14	0.47
1:A:77:LYS:O	1:A:81:ILE:HG13	2.14	0.47
1:B:64:ARG:HB3	1:B:69:GLU:HA	1.96	0.47
1:A:370:GLU:HG2	1:A:371:VAL:N	2.28	0.47
1:A:273:LEU:HB2	1:A:310:TYR:HB2	1.95	0.47
1:B:169:LEU:HG	1:B:443:ILE:CG2	2.44	0.47
1:A:219:TYR:CZ	1:A:280:PRO:HD2	2.49	0.47
1:A:105:ARG:NH1	1:A:105:ARG:CG	2.74	0.47
1:A:207:LEU:N	1:A:207:LEU:HD22	2.28	0.47
1:A:208:ILE:HG12	1:A:214:PRO:HD3	1.96	0.47
1:A:303:HIS:HB2	1:A:410:THR:OG1	2.14	0.47
1:A:2:LEU:HD12	1:A:106:LEU:HB3	1.96	0.47
1:B:111:HIS:CD2	1:B:112:PRO:HD2	2.49	0.47
1:A:307:GLN:OE1	1:A:323:ILE:HG22	2.15	0.46
1:B:239:ILE:O	1:B:284:LYS:HE3	2.15	0.46
1:B:252:THR:C	1:B:254:GLU:H	2.19	0.46
1:B:427:THR:HG22	1:B:445:PRO:CD	2.42	0.46
1:B:75:LEU:O	1:B:75:LEU:HD13	2.15	0.46
1:A:435:TRP:CH2	1:A:441:LYS:HD3	2.51	0.46
1:A:64:ARG:HB3	1:A:69:GLU:HA	1.98	0.46
1:A:358:ILE:HB	1:A:372:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD22	1:A:380:TRP:HB2	1.80	0.46
1:A:395:GLU:HB2	1:A:396:LYS:H	1.51	0.46
1:A:59:VAL:O	1:A:63:LYS:HD3	2.15	0.46
1:B:288:THR:HG21	1:B:298:ARG:CD	2.29	0.46
1:A:39:GLU:HB2	1:A:95:LEU:HD21	1.97	0.46
1:A:51:ARG:HG2	1:A:54:ARG:NH2	2.31	0.45
1:A:333:GLU:O	1:A:433:VAL:HG21	2.17	0.45
1:A:343:ILE:HD11	1:A:357:ASP:OD2	2.16	0.45
1:B:250:ILE:O	1:B:250:ILE:HG13	2.14	0.45
1:B:267:ASP:OD2	1:B:269:LYS:HB2	2.16	0.45
1:B:329:GLU:O	1:B:333:GLU:HG3	2.17	0.45
1:A:288:THR:O	1:A:288:THR:HG23	2.16	0.45
1:A:62:GLY:O	1:A:65:ARG:HB3	2.17	0.45
1:B:191:GLU:HG3	1:B:443:ILE:CG2	2.46	0.45
1:B:325:ARG:HH11	1:B:325:ARG:HG2	1.82	0.45
1:A:207:LEU:N	1:A:207:LEU:CD2	2.79	0.45
1:A:396:LYS:HZ2	1:A:396:LYS:HA	1.81	0.45
1:B:306:GLU:HG3	1:B:307:GLN:N	2.31	0.45
1:B:429:ARG:NH2	1:B:442:GLU:OE1	2.49	0.45
1:A:269:LYS:CE	1:A:269:LYS:HA	2.37	0.45
1:A:368:PHE:O	1:A:369:ARG:HD2	2.17	0.45
1:B:355:LYS:HE3	1:B:373:SER:OG	2.17	0.45
1:A:101:TYR:O	1:A:105:ARG:HG3	2.17	0.44
1:B:40:TRP:HE1	1:B:96:LYS:CE	2.28	0.44
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.81	0.44
1:A:21:ARG:HH21	1:A:21:ARG:HG2	1.82	0.44
1:A:253:ALA:O	1:A:257:LEU:HB2	2.16	0.44
1:A:432:LYS:HG2	1:A:435:TRP:CH2	2.53	0.44
1:A:1:MET:H1	1:A:384:ARG:HH21	1.65	0.44
1:A:94:GLU:OE1	1:A:94:GLU:HA	2.18	0.44
1:A:447:GLU:O	1:A:448:LYS:CB	2.63	0.44
1:B:61:ILE:HB	1:B:74:LEU:CD2	2.48	0.44
1:B:68:GLY:C	1:B:70:PRO:HD3	2.38	0.44
1:B:92:VAL:CG1	1:B:96:LYS:HE3	2.47	0.44
1:A:257:LEU:HA	1:A:257:LEU:HD12	1.91	0.44
1:A:67:LYS:HG2	1:A:68:GLY:H	1.81	0.44
1:B:221:VAL:HG21	1:B:225:VAL:HG22	1.99	0.44
1:A:333:GLU:HB3	1:A:433:VAL:HG21	1.99	0.44
1:B:1:MET:H3	1:B:384:ARG:HD2	1.83	0.44
1:B:21:ARG:CG	1:B:21:ARG:HH21	2.30	0.44
1:B:274:LEU:HD12	1:B:309:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:O	1:A:149:LYS:HG3	2.17	0.44
1:A:108:ASN:ND2	1:A:380:TRP:HB2	2.33	0.44
1:A:147:GLN:C	1:A:149:LYS:H	2.20	0.44
1:B:242:VAL:HG11	1:B:247:LEU:HB2	1.99	0.43
1:A:105:ARG:NH1	1:A:105:ARG:HG2	2.28	0.43
1:B:127:ARG:CZ	1:B:325:ARG:HH12	2.32	0.43
1:B:52:HIS:CD2	1:B:56:LYS:HE3	2.53	0.43
1:A:184:ARG:HH21	1:A:184:ARG:HG2	1.83	0.43
1:A:126:ILE:CG1	1:A:340:VAL:HG23	2.49	0.43
1:A:374:ALA:HA	1:A:405:SER:HB2	2.00	0.43
1:B:323:ILE:HD12	1:B:405:SER:HB2	2.00	0.43
1:A:343:ILE:HD12	1:A:355:LYS:HG2	2.01	0.43
1:B:269:LYS:N	1:B:269:LYS:HD2	2.32	0.43
1:A:2:LEU:HA	1:A:2:LEU:HD23	1.72	0.43
1:B:252:THR:C	1:B:254:GLU:N	2.72	0.43
1:A:158:LYS:HA	1:A:159:PRO:HD3	1.89	0.43
1:B:77:LYS:O	1:B:81:ILE:HG13	2.18	0.43
1:B:115:PRO:HD3	1:B:342:ASN:HD21	1.82	0.43
1:B:242:VAL:HG12	1:B:247:LEU:O	2.19	0.43
1:B:168:ILE:O	1:B:446:VAL:HG22	2.19	0.43
1:A:204:LEU:HA	1:A:204:LEU:HD12	1.71	0.42
1:A:68:GLY:C	1:A:70:PRO:HD3	2.39	0.42
1:A:208:ILE:HD11	1:A:214:PRO:HG3	2.00	0.42
1:A:306:GLU:HG3	1:A:307:GLN:N	2.34	0.42
1:A:429:ARG:NH1	1:A:442:GLU:OE1	2.50	0.42
1:B:191:GLU:HB2	1:B:443:ILE:CD1	2.49	0.42
1:A:1:MET:N	1:A:384:ARG:HH21	2.16	0.42
1:B:282:PHE:HA	1:B:300:HIS:O	2.19	0.42
1:A:378:THR:OG1	1:A:379:ASP:N	2.52	0.42
1:B:188:LEU:HG	1:B:192:ILE:HG22	2.01	0.42
1:A:249:LEU:HD11	1:B:249:LEU:HD21	2.01	0.42
1:A:50:LEU:HD22	1:A:81:ILE:HG23	2.02	0.42
1:A:432:LYS:HA	1:A:435:TRP:CE2	2.55	0.42
1:B:124:VAL:HA	1:B:125:PRO:HD3	1.91	0.42
1:B:429:ARG:HG2	1:B:429:ARG:HH21	1.84	0.42
1:B:132:ALA:HB1	1:B:361:TRP:CD1	2.55	0.42
1:A:222:ARG:HG3	1:A:246:ASP:CG	2.40	0.42
1:A:206:ARG:NH2	1:A:333:GLU:OE1	2.51	0.41
1:B:429:ARG:HG2	1:B:429:ARG:NH2	2.34	0.41
1:A:269:LYS:HE2	1:A:269:LYS:CA	2.40	0.41
1:A:343:ILE:HD11	1:A:357:ASP:CG	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:O	1:A:47:ILE:HG13	2.19	0.41
1:B:389:PHE:CD1	1:B:400:VAL:HG12	2.54	0.41
1:B:365:GLN:HG3	1:B:419:GLU:OE1	2.21	0.41
1:B:61:ILE:HD12	1:B:75:LEU:HD23	2.01	0.41
1:A:354:LYS:HE2	1:A:356:TYR:CZ	2.55	0.41
1:B:11:PRO:HB3	1:B:34:LEU:HD11	2.01	0.41
1:A:2:LEU:HD12	1:A:106:LEU:CB	2.51	0.41
1:A:73:GLU:O	1:A:76:ALA:HB3	2.20	0.41
1:B:360:ALA:HB3	1:B:362:MET:CE	2.50	0.41
1:B:390:ARG:CD	1:B:393:THR:HA	2.51	0.41
1:A:120:GLU:CD	1:A:120:GLU:H	2.24	0.41
1:A:243:GLU:OE1	1:B:241:LYS:HD3	2.20	0.41
1:A:186:TYR:CD2	1:A:188:LEU:HD13	2.56	0.41
1:A:320:HIS:HA	1:A:403:LEU:HD23	2.01	0.41
1:A:335:GLU:HB2	1:A:421:HIS:CE1	2.55	0.41
1:B:271:LEU:HA	1:B:271:LEU:HD12	1.88	0.41
1:A:358:ILE:CG1	1:A:372:VAL:HG22	2.51	0.41
1:A:242:VAL:CG2	1:A:245:GLU:HB2	2.50	0.41
1:A:69:GLU:C	1:A:71:VAL:H	2.25	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.86	0.41
1:A:21:ARG:NH2	1:A:21:ARG:HG2	2.36	0.40
1:A:26:LYS:O	1:A:29:TRP:HB2	2.20	0.40
1:A:281:CYS:O	1:A:301:GLN:HA	2.21	0.40
1:A:369:ARG:HH21	1:A:369:ARG:HG3	1.86	0.40
1:A:297:PHE:CD1	1:A:412:ARG:HG2	2.56	0.40
1:B:323:ILE:HD12	1:B:405:SER:CB	2.52	0.40
1:A:324:ILE:O	1:A:328:GLU:HG3	2.22	0.40
1:A:371:VAL:CG1	1:A:372:VAL:HG13	2.46	0.40
1:A:95:LEU:O	1:A:99:ILE:HG13	2.21	0.40
1:B:127:ARG:HB2	1:B:340:VAL:HG13	2.04	0.40
1:B:3:ASP:HB2	1:B:383:ARG:CZ	2.51	0.40
1:B:8:ARG:NH2	1:B:37:ASP:OD1	2.54	0.40
1:A:215:VAL:HB	1:B:189:LEU:HD23	2.03	0.40
1:B:8:ARG:HA	1:B:34:LEU:HD21	2.03	0.40
1:A:8:ARG:NH2	1:A:37:ASP:OD1	2.54	0.40
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.86	0.40
1:B:101:TYR:C	1:B:101:TYR:CD2	2.94	0.40
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.87	0.40
1:B:314:GLU:CD	1:B:314:GLU:H	2.24	0.40

There are no symmetry-related clashes.

## 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	446/455 (98%)	409 (92%)	31 (7%)	6 (1%)	12	45
1	B	446/455 (98%)	414 (93%)	30 (7%)	2 (0%)	34	72
All	All	892/910 (98%)	823 (92%)	61 (7%)	8 (1%)	17	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	LYS
1	A	190	ASN
1	B	294	LYS
1	A	447	GLU
1	A	25	GLU
1	A	396	LYS
1	B	71	VAL
1	A	71	VAL

### 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	399/405 (98%)	372 (93%)	27 (7%)	16	48
1	B	399/405 (98%)	367 (92%)	32 (8%)	12	40
All	All	798/810 (98%)	739 (93%)	59 (7%)	13	44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	LEU
1	A	13	LEU
1	A	17	ASP
1	A	44	LEU
1	A	49	ARG
1	A	54	ARG
1	A	63	LYS
1	A	119	ASP
1	A	188	LEU
1	A	191	GLU
1	A	204	LEU
1	A	215	VAL
1	A	217	PRO
1	A	225	VAL
1	A	238	VAL
1	A	252	THR
1	A	257	LEU
1	A	269	LYS
1	A	278	VAL
1	A	306	GLU
1	A	312	ARG
1	A	334	LEU
1	A	371	VAL
1	A	396	LYS
1	A	429	ARG
1	A	447	GLU
1	B	2	LEU
1	B	6	LEU
1	B	14	VAL
1	B	44	LEU
1	B	48	ASN
1	B	72	ASP
1	B	75	LEU
1	B	106	LEU
1	B	139	LEU
1	B	168	ILE
1	B	169	LEU
1	B	188	LEU
1	B	191	GLU
1	B	204	LEU
1	B	206	ARG
1	B	215	VAL

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Mol	Chain	Res	Type
1	B	217	PRO
1	B	230	THR
1	B	257	LEU
1	B	269	LYS
1	B	271	LEU
1	B	274	LEU
1	B	293	THR
1	B	294	LYS
1	B	301	GLN
1	B	306	GLU
1	B	340	VAL
1	B	341	VAL
1	B	392	ARG
1	B	393	THR
1	B	394	ASP
1	B	427	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	147	GLN
1	B	16	ASN
1	B	48	ASN
1	B	138	HIS
1	B	342	ASN

### 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

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	448/455 (98%)	-0.18	2 (0%) 92 79	39, 70, 118, 163	0
1	B	448/455 (98%)	-0.21	10 (2%) 62 33	36, 64, 126, 175	0
All	All	896/910 (98%)	-0.20	12 (1%) 77 51	36, 68, 124, 175	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	GLY	3.5
1	B	61	ILE	3.2
1	B	69	GLU	3.0
1	B	66	LYS	3.0
1	B	60	GLU	2.5
1	B	63	LYS	2.4
1	B	70	PRO	2.4
1	B	65	ARG	2.4
1	B	67	LYS	2.4
1	A	65	ARG	2.3
1	B	448	LYS	2.3
1	A	69	GLU	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.