



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:20 pm GMT

PDB ID : 2UXT  
Title : SufI Protein from Escherichia Coli  
Authors : Tarry, M.J.; Roversi, P.; Sargent, F.; Berks, B.C.; Lea, S.M.  
Deposited on : 2007-03-29  
Resolution : 1.90 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 : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

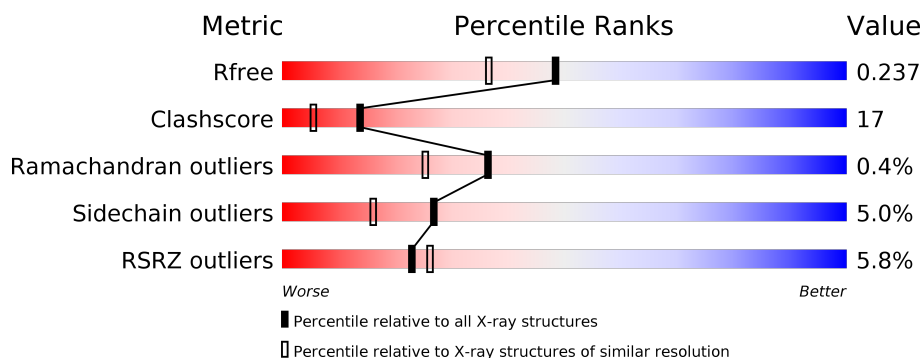
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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	451	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	B	451	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7014 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 PROTEIN SUFI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3313	2103	589	607	14			
1	B	420	Total	C	N	O	S	0	0	0
			3295	2095	580	606	14			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	229	Total	O	0	0
			229	229		
2	B	177	Total	O	0	0
			177	177		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.47Å 89.55Å 153.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 1.90 39.80 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.84-1.90) 98.0 (39.80-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.89Å)	Xtriage
Refinement program	TNT 5.13.1.0	Depositor
R, $R_{free}$	0.191 , (Not available) 0.198 , 0.237	Depositor DCC
$R_{free}$ test set	2976 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	0.32	0/3402	0.63	1/4645 (0.0%)
1	B	0.33	0/3382	0.61	1/4619 (0.0%)
All	All	0.32	0/6784	0.62	2/9264 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	LEU	C-N-CD	-13.22	91.52	120.60
1	B	71	ASN	N-CA-C	6.37	128.21	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	3313	0	3262	105	0
1	B	3295	0	3243	121	0
2	A	229	0	0	8	0
2	B	177	0	0	5	0
All	All	7014	0	6505	223	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 17.

All (223) 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:347:ALA:HB1	1:B:433:LEU:HD23	1.20	1.12
1:A:312:SER:HA	1:A:314:ILE:H	1.25	1.00
1:B:40:LEU:HD22	1:B:77:PRO:HB2	1.46	0.95
1:A:312:SER:N	1:A:313:SER:HB3	1.82	0.93
1:B:58:SER:HB2	1:B:60:THR:HG23	1.54	0.89
1:B:212:LEU:HD12	1:B:315:LEU:HD13	1.57	0.87
1:A:282:LEU:HD12	1:A:336:LEU:HD22	1.54	0.86
1:B:347:ALA:HB1	1:B:433:LEU:CD2	2.06	0.85
1:B:148:ARG:HH11	1:B:148:ARG:HG2	1.41	0.84
1:A:312:SER:HA	1:A:314:ILE:N	1.93	0.84
1:B:266:VAL:HG11	1:B:415:PRO:HB2	1.60	0.84
1:A:228:TRP:CZ3	1:A:336:LEU:HD21	2.12	0.84
1:A:282:LEU:CD1	1:A:336:LEU:HD22	2.08	0.82
1:A:287:ASN:HB3	2:A:2134:HOH:O	1.81	0.80
1:B:35:PRO:HD3	1:B:217:VAL:HG11	1.66	0.78
1:B:380:GLN:OE1	1:B:469:VAL:HG22	1.84	0.77
1:B:50:MET:HG3	1:B:70:ILE:HG21	1.68	0.76
1:A:257:GLY:HA2	2:A:2205:HOH:O	1.85	0.76
1:A:64:ARG:HD3	1:A:194:PHE:CD1	2.21	0.76
1:B:347:ALA:CB	1:B:433:LEU:HD23	2.09	0.74
1:A:65:ALA:HB3	1:A:196:THR:HG21	1.69	0.74
1:B:40:LEU:CD2	1:B:77:PRO:HB2	2.19	0.73
1:A:345:ILE:CD1	1:A:420:TRP:HE1	2.02	0.73
1:B:341:LEU:CD1	1:B:345:ILE:HD11	2.19	0.73
1:B:148:ARG:NH1	1:B:148:ARG:HG2	2.01	0.73
1:B:212:LEU:CD1	1:B:315:LEU:HD13	2.18	0.72
1:A:312:SER:HA	1:A:314:ILE:HD12	1.71	0.72
1:A:345:ILE:HD11	1:A:420:TRP:HE1	1.53	0.72
1:A:379:GLN:O	1:A:382:THR:HG22	1.89	0.71
1:A:35:PRO:HD3	1:A:217:VAL:HG11	1.73	0.71
1:B:50:MET:CE	1:B:79:ILE:HD11	2.21	0.70
1:B:89:LEU:HD23	1:B:91:TYR:CE1	2.27	0.70
1:A:345:ILE:HD11	1:A:420:TRP:NE1	2.07	0.70
1:A:42:SER:O	1:A:43:ARG:HB2	1.90	0.70
1:B:40:LEU:HD22	1:B:77:PRO:CB	2.21	0.69
1:A:287:ASN:O	1:A:287:ASN:ND2	2.26	0.69
1:A:312:SER:CA	1:A:314:ILE:H	2.04	0.68
1:B:245:GLN:HG2	1:B:270:GLN:HG3	1.75	0.68
1:A:226:ARG:HD3	1:A:329:LEU:CD2	2.24	0.67
1:A:257:GLY:HA3	1:A:260:GLY:O	1.95	0.66
1:B:257:GLY:HA2	2:B:2160:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:SER:HB2	1:B:60:THR:CG2	2.24	0.66
1:A:289:ASP:HB2	2:A:2134:HOH:O	1.94	0.65
1:B:50:MET:HE3	1:B:70:ILE:HG21	1.79	0.64
1:B:341:LEU:HD23	1:B:342:PRO:HD2	1.78	0.64
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.63	0.64
1:B:32:GLN:HB2	1:B:217:VAL:HG21	1.80	0.62
1:A:228:TRP:CE3	1:A:336:LEU:HD21	2.34	0.62
1:A:414:PHE:CE2	1:B:251:PRO:HB3	2.34	0.62
1:A:258:ASP:HB2	1:A:421:LYS:HA	1.81	0.62
1:A:312:SER:CA	1:A:313:SER:HB3	2.29	0.62
1:B:395:ALA:HB3	1:B:451:GLN:HB2	1.81	0.62
1:B:148:ARG:HA	2:B:2176:HOH:O	1.98	0.62
1:B:50:MET:HG3	1:B:70:ILE:CG2	2.30	0.62
1:A:63:THR:HG21	2:A:2022:HOH:O	1.98	0.61
1:B:406:ARG:HD3	1:B:433:LEU:CD2	2.30	0.61
1:A:226:ARG:HD3	1:A:329:LEU:HD21	1.81	0.61
1:B:49:PHE:CZ	1:B:90:ILE:HD12	2.36	0.61
1:B:380:GLN:CD	1:B:469:VAL:HG22	2.20	0.61
1:A:336:LEU:HB3	1:A:337:PRO:CD	2.32	0.60
1:A:406:ARG:HD2	1:A:433:LEU:HB2	1.84	0.60
1:A:289:ASP:O	1:A:325:PRO:HG2	2.02	0.60
1:A:30:GLN:HG3	2:A:2140:HOH:O	2.01	0.59
1:B:406:ARG:HH11	1:B:433:LEU:CD2	2.15	0.59
1:B:212:LEU:HD12	1:B:315:LEU:CD1	2.31	0.59
1:A:355:ASP:OD2	1:A:389:ARG:NH1	2.35	0.59
1:A:287:ASN:OD1	1:B:410:GLY:HA3	2.02	0.58
1:B:406:ARG:HD3	1:B:433:LEU:HD22	1.84	0.58
1:A:406:ARG:CD	1:A:433:LEU:HB2	2.33	0.58
1:B:146:PRO:O	1:B:147:ASN:HB2	2.03	0.58
1:B:268:VAL:HG21	1:B:271:LEU:HD13	1.86	0.58
1:A:266:VAL:HG11	1:A:415:PRO:HB2	1.85	0.58
1:B:68:TRP:CE3	1:B:95:LEU:HD13	2.38	0.58
1:B:406:ARG:NH1	2:B:2149:HOH:O	2.29	0.57
1:B:339:ARG:CG	1:B:339:ARG:HH11	2.18	0.57
1:B:458:ARG:HD3	2:B:2070:HOH:O	2.05	0.57
1:A:312:SER:CB	1:A:314:ILE:HD13	2.35	0.56
1:A:395:ALA:HB3	1:A:451:GLN:HB2	1.85	0.56
1:A:285:MET:CE	1:A:325:PRO:HG3	2.35	0.56
1:A:62:GLY:N	1:A:196:THR:OG1	2.38	0.56
1:A:323:LEU:O	1:A:325:PRO:HD3	2.06	0.56
1:B:59:PHE:O	1:B:60:THR:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HG2	1:A:148:ARG:NH1	2.19	0.56
1:A:325:PRO:HB2	2:A:2142:HOH:O	2.07	0.55
1:B:35:PRO:HD3	1:B:217:VAL:CG1	2.36	0.55
1:B:369:TRP:CZ2	1:B:371:VAL:HG12	2.42	0.55
1:A:212:LEU:HD21	1:A:242:TYR:HE2	1.72	0.55
1:A:46:GLN:HB3	1:A:47:PRO:HD2	1.88	0.55
1:A:39:LEU:HD21	1:A:80:ARG:CZ	2.37	0.55
1:B:224:VAL:O	1:B:325:PRO:HA	2.07	0.55
1:B:50:MET:HE1	1:B:77:PRO:HG2	1.88	0.55
1:A:382:THR:HG21	2:A:2180:HOH:O	2.07	0.53
1:A:385:ARG:HH11	1:A:406:ARG:HH22	1.56	0.53
1:B:68:TRP:CZ3	1:B:95:LEU:HD13	2.43	0.53
1:B:341:LEU:HD13	1:B:345:ILE:HD11	1.90	0.53
1:A:312:SER:HB2	1:A:314:ILE:HD13	1.91	0.52
1:A:312:SER:CA	1:A:314:ILE:HD12	2.37	0.52
1:B:258:ASP:HB2	1:B:421:LYS:HA	1.92	0.52
1:B:241:ARG:HD2	1:B:425:TRP:CE2	2.44	0.52
1:B:50:MET:HE1	1:B:79:ILE:HD11	1.91	0.52
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.74	0.52
1:A:154:TYR:O	1:A:189:LYS:NZ	2.43	0.52
1:A:245:GLN:HA	1:A:252:LEU:HD11	1.92	0.52
1:B:63:THR:HG21	1:B:195:GLY:HA3	1.91	0.52
1:B:257:GLY:HA3	1:B:260:GLY:O	2.10	0.52
1:A:35:PRO:CD	1:A:217:VAL:HG11	2.40	0.51
1:B:341:LEU:HD23	1:B:342:PRO:CD	2.40	0.51
1:A:352:ARG:HD3	1:A:354:ARG:NH2	2.26	0.51
1:B:49:PHE:CE2	1:B:90:ILE:HD12	2.46	0.51
1:B:69:GLY:HA3	1:B:73:ARG:O	2.11	0.51
1:A:352:ARG:HD3	1:A:354:ARG:CZ	2.40	0.51
1:B:402:MET:HE3	1:B:420:TRP:CE2	2.45	0.51
1:A:146:PRO:O	1:A:147:ASN:HB2	2.09	0.51
1:A:336:LEU:HB3	1:A:337:PRO:HD2	1.93	0.50
1:B:74:TYR:O	1:B:75:LEU:HB2	2.10	0.50
1:B:383:TRP:CH2	1:B:420:TRP:HH2	2.30	0.50
1:A:64:ARG:HD3	1:A:194:PHE:CE1	2.47	0.50
1:B:68:TRP:CD2	1:B:95:LEU:HD13	2.46	0.50
1:A:282:LEU:HD13	1:A:336:LEU:HD22	1.93	0.50
1:A:226:ARG:NH2	1:A:329:LEU:HD21	2.26	0.50
1:A:74:TYR:O	1:A:75:LEU:HB2	2.12	0.49
1:A:212:LEU:HD21	1:A:242:TYR:CE2	2.47	0.49
1:A:148:ARG:CG	1:A:148:ARG:HH11	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLN:NE2	1:B:270:GLN:HE21	2.11	0.49
1:B:52:VAL:HG22	1:B:93:ASN:HA	1.96	0.48
1:A:224:VAL:HG21	1:A:285:MET:HG3	1.94	0.48
1:B:354:ARG:O	1:B:387:THR:HG22	2.14	0.47
1:B:421:LYS:HE3	1:B:423:THR:O	2.13	0.47
1:A:379:GLN:HE21	1:A:469:VAL:CG2	2.28	0.47
1:B:208:VAL:CG1	1:B:240:ARG:NH2	2.77	0.47
1:B:355:ASP:OD1	1:B:389:ARG:NH2	2.35	0.47
1:B:404:GLN:HG2	1:B:406:ARG:HD2	1.97	0.47
1:B:50:MET:HE2	1:B:141:TYR:CZ	2.50	0.47
1:A:226:ARG:HD3	1:A:329:LEU:HD22	1.96	0.46
1:A:354:ARG:HG3	1:A:386:TRP:NE1	2.29	0.46
1:A:69:GLY:HA3	1:A:73:ARG:O	2.14	0.46
1:A:389:ARG:HD3	1:A:429:GLN:OE1	2.15	0.46
1:B:35:PRO:CD	1:B:217:VAL:CG1	2.93	0.46
1:B:98:ASN:HB3	1:B:119:MET:HG2	1.97	0.46
1:A:263:PRO:HA	1:A:341:LEU:HB2	1.97	0.46
1:B:82:TRP:CH2	1:B:169:LYS:HD2	2.51	0.46
1:B:354:ARG:CZ	1:B:376:VAL:HG13	2.46	0.46
1:B:355:ASP:HA	1:B:387:THR:HG23	1.98	0.45
1:A:335:SER:N	1:A:336:LEU:CA	2.80	0.45
1:B:98:ASN:HB2	1:B:119:MET:CE	2.46	0.45
1:A:389:ARG:HG2	1:A:429:GLN:HG3	1.97	0.45
1:A:385:ARG:NH1	1:A:406:ARG:HH22	2.13	0.45
1:B:119:MET:CE	1:B:145:THR:HG23	2.46	0.45
1:B:402:MET:CE	1:B:420:TRP:CE2	2.99	0.45
1:B:194:PHE:CD1	1:B:194:PHE:N	2.84	0.45
1:B:63:THR:OG1	1:B:194:PHE:O	2.26	0.45
1:B:328:LEU:N	1:B:328:LEU:HD13	2.31	0.45
1:B:339:ARG:CG	1:B:339:ARG:NH1	2.78	0.45
1:B:389:ARG:HG2	1:B:429:GLN:HB2	1.98	0.45
1:A:385:ARG:HH11	1:A:406:ARG:NH2	2.13	0.45
1:B:50:MET:CE	1:B:141:TYR:CZ	3.00	0.45
1:B:98:ASN:CB	1:B:119:MET:HE3	2.47	0.44
1:A:226:ARG:HH21	1:A:329:LEU:HD21	1.81	0.44
1:B:98:ASN:CB	1:B:119:MET:CE	2.95	0.44
1:B:369:TRP:CZ2	1:B:371:VAL:CG1	3.00	0.44
1:B:50:MET:O	1:B:91:TYR:HA	2.18	0.44
1:A:223:GLU:HA	1:A:324:ARG:O	2.18	0.44
1:B:100:SER:OG	1:B:145:THR:HA	2.17	0.44
1:A:75:LEU:HA	1:A:156:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:H	1:B:40:LEU:HD23	1.82	0.44
1:A:35:PRO:CD	1:A:217:VAL:CG1	2.95	0.44
1:B:412:MET:HB3	1:B:412:MET:HE2	1.85	0.44
1:A:89:LEU:O	1:A:127:ALA:HA	2.18	0.44
1:B:383:TRP:HH2	1:B:420:TRP:HH2	1.65	0.44
1:B:469:VAL:O	1:B:470:PRO:O	2.36	0.44
1:B:71:ASN:N	1:B:72:GLY:HA2	2.33	0.44
1:A:122:PRO:O	1:A:123:ASN:HB2	2.17	0.44
1:B:103:VAL:HG12	1:B:106:LEU:HB2	2.00	0.43
1:B:68:TRP:CE3	1:B:95:LEU:CD1	3.01	0.43
1:A:312:SER:OG	1:A:314:ILE:HB	2.18	0.43
1:B:97:GLU:CD	1:B:148:ARG:HE	2.21	0.43
1:B:261:PHE:O	1:B:341:LEU:HD12	2.19	0.43
1:B:201:GLU:CG	1:B:458:ARG:HH21	2.31	0.43
1:B:287:ASN:OD1	1:B:289:ASP:HB2	2.19	0.43
1:B:89:LEU:HD21	1:B:91:TYR:CZ	2.54	0.43
1:A:212:LEU:HD11	1:A:295:CYS:SG	2.58	0.43
1:A:271:LEU:HD21	1:A:279:ARG:HD2	2.01	0.43
1:B:339:ARG:NH2	1:B:344:GLU:OE2	2.51	0.43
1:B:343:THR:OG1	1:B:344:GLU:N	2.51	0.43
1:A:251:PRO:HB3	1:B:414:PHE:CE2	2.53	0.43
1:A:232:ARG:HG2	1:A:280:GLU:HG2	2.01	0.42
1:A:292:SER:HB3	1:A:319:LEU:CD1	2.50	0.42
1:A:285:MET:HE2	1:A:325:PRO:HG3	2.01	0.42
1:B:406:ARG:HD3	1:B:433:LEU:HD23	2.01	0.42
1:B:208:VAL:HG13	1:B:240:ARG:NH2	2.34	0.42
1:B:241:ARG:HD2	1:B:425:TRP:CZ2	2.55	0.42
1:A:312:SER:CB	1:A:314:ILE:CD1	2.98	0.42
1:B:89:LEU:CD2	1:B:91:TYR:CE1	2.99	0.42
1:B:148:ARG:HH11	1:B:148:ARG:CG	2.17	0.42
1:A:113:MET:HB2	1:A:114:GLY:HA2	2.01	0.42
1:A:290:GLU:HG2	1:A:291:VAL:N	2.35	0.42
1:A:42:SER:OG	1:A:43:ARG:N	2.53	0.42
1:B:89:LEU:CD2	1:B:91:TYR:CZ	3.03	0.42
1:B:50:MET:CE	1:B:79:ILE:CD1	2.95	0.42
1:A:65:ALA:HB3	1:A:196:THR:CG2	2.45	0.41
1:B:63:THR:CG2	1:B:195:GLY:HA3	2.50	0.41
1:A:285:MET:HE3	1:A:325:PRO:HG3	2.02	0.41
1:A:345:ILE:HD11	1:A:420:TRP:CE2	2.54	0.41
1:A:109:PRO:HD2	1:A:112:LEU:HD12	2.03	0.41
1:A:262:LEU:O	1:A:340:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HB3	1:A:88:LYS:CG	2.50	0.41
1:A:48:LEU:HB2	1:A:89:LEU:HD12	2.02	0.41
1:A:50:MET:CE	1:A:79:ILE:HD11	2.49	0.41
1:B:440:SER:HB3	1:B:446:PHE:CE2	2.56	0.41
1:B:98:ASN:OD1	1:B:121:SER:HA	2.21	0.41
1:B:68:TRP:CH2	1:B:95:LEU:HD13	2.56	0.41
1:B:395:ALA:CB	1:B:451:GLN:HB2	2.49	0.41
1:A:154:TYR:CD2	1:A:199:TYR:HB2	2.57	0.40
1:A:295:CYS:O	1:A:318:THR:OG1	2.28	0.40
1:A:292:SER:HB3	1:A:319:LEU:HD11	2.02	0.40
1:B:233:LEU:O	1:B:278:ARG:HA	2.21	0.40
1:B:412:MET:HA	1:B:413:PRO:HD3	1.91	0.40
1:B:314:ILE:HG12	1:B:314:ILE:H	1.60	0.40
1:B:335:SER:HA	2:B:2111:HOH:O	2.21	0.40
1:B:58:SER:CB	1:B:60:THR:HG23	2.39	0.40
1:A:73:ARG:HD2	2:A:2026:HOH:O	2.20	0.40
1:B:341:LEU:CD2	1:B:343:THR:CG2	2.98	0.40
1:A:115:GLY:HA3	1:A:116:PRO:HD2	1.90	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	416/451 (92%)	395 (95%)	18 (4%)	3 (1%)	24	13
1	B	412/451 (91%)	393 (95%)	19 (5%)	0	100	100
All	All	828/902 (92%)	788 (95%)	37 (4%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	61	PRO
1	A	64	ARG

### 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	363/386 (94%)	348 (96%)	15 (4%)	33	23
1	B	362/386 (94%)	341 (94%)	21 (6%)	22	12
All	All	725/772 (94%)	689 (95%)	36 (5%)	27	16

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	43	ARG
1	A	44	ARG
1	A	64	ARG
1	A	66	SER
1	A	87	VAL
1	A	125	ASP
1	A	204	SER
1	A	241	ARG
1	A	278	ARG
1	A	287	ASN
1	A	290	GLU
1	A	345	ILE
1	A	389	ARG
1	A	391	ASP
1	B	42	SER
1	B	58	SER
1	B	66	SER
1	B	121	SER
1	B	125	ASP
1	B	196	THR

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Mol	Chain	Res	Type
1	B	212	LEU
1	B	213	LEU
1	B	225	SER
1	B	278	ARG
1	B	313	SER
1	B	314	ILE
1	B	315	LEU
1	B	328	LEU
1	B	333	THR
1	B	339	ARG
1	B	346	MET
1	B	387	THR
1	B	406	ARG
1	B	433	LEU
1	B	469	VAL

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	107	GLN
1	A	372	ASN
1	A	449	ASN
1	B	245	GLN
1	B	367	GLN
1	B	449	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

### 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	422/451 (93%)	0.16	24 (5%) 24 27	15, 26, 50, 72	0
1	B	420/451 (93%)	0.47	25 (5%) 22 25	18, 29, 52, 78	0
All	All	842/902 (93%)	0.32	49 (5%) 23 26	15, 27, 51, 78	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	VAL	8.1
1	B	314	ILE	7.3
1	A	57	TRP	6.1
1	A	43	ARG	6.0
1	B	328	LEU	5.9
1	B	315	LEU	5.6
1	A	345	ILE	5.5
1	A	63	THR	5.2
1	A	62	GLY	5.2
1	B	194	PHE	5.2
1	B	470	PRO	5.1
1	B	316	VAL	5.0
1	A	471	ARG	5.0
1	A	65	ALA	4.6
1	A	312	SER	4.6
1	A	61	PRO	4.5
1	B	200	ASN	4.4
1	B	60	THR	4.4
1	B	313	SER	4.1
1	A	336	LEU	4.0
1	B	64	ARG	3.9
1	A	64	ARG	3.6
1	A	287	ASN	3.6
1	A	343	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	204	SER	3.4
1	B	62	GLY	3.4
1	B	63	THR	3.1
1	B	347	ALA	2.9
1	A	195	GLY	2.8
1	B	193	ASN	2.8
1	A	44	ARG	2.8
1	B	343	THR	2.7
1	A	289	ASP	2.7
1	A	338	MET	2.7
1	A	325	PRO	2.6
1	B	192	ASP	2.6
1	A	30	GLN	2.6
1	B	338	MET	2.6
1	A	346	MET	2.4
1	A	335	SER	2.3
1	B	317	SER	2.3
1	B	468	PRO	2.2
1	B	341	LEU	2.2
1	B	327	GLY	2.2
1	A	42	SER	2.2
1	B	43	ARG	2.2
1	A	329	LEU	2.1
1	B	342	PRO	2.1
1	A	203	GLY	2.1

## 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.