Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:08 am BST

PDB ID	:	1SRU
Title	:	Crystal structure of full length E. coli SSB protein
Authors	:	Savvides, S.N.; Raghunathan, S.; Fuetterer, K.; Kozlov, A.G.; Lohman, T.M.; Waksman, G.
Deposited on	:	2004-03-23
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

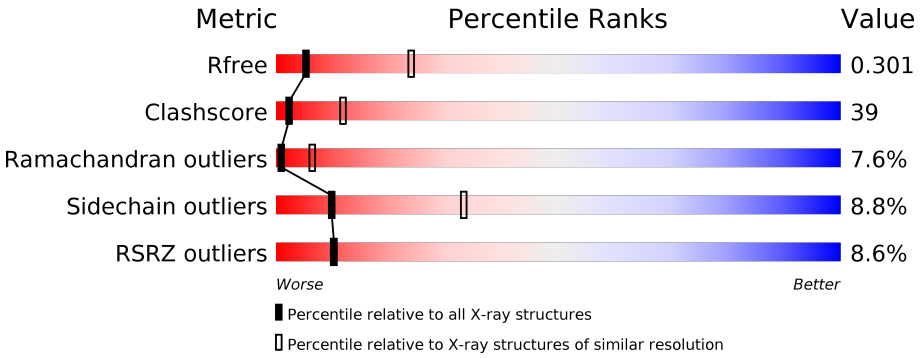
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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 <=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	113	8% 42% 41% 5% 12%
1	B	113	3% 40% 35% 8% • 14%
1	C	113	10% 39% 32% 12% • 15%
1	D	113	10% 33% 48% 8% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2808 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 Single-strand binding protein.

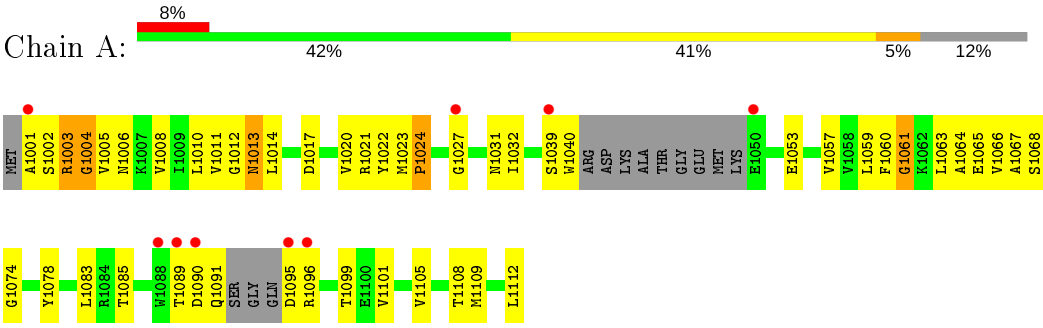
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			698	440	122	134	2			
1	B	97	Total	C	N	O	S	0	0	0
			688	432	121	134	1			
1	C	96	Total	C	N	O	S	0	0	0
			698	443	121	133	1			
1	D	101	Total	C	N	O	S	0	0	0
			724	453	125	144	2			

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 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.

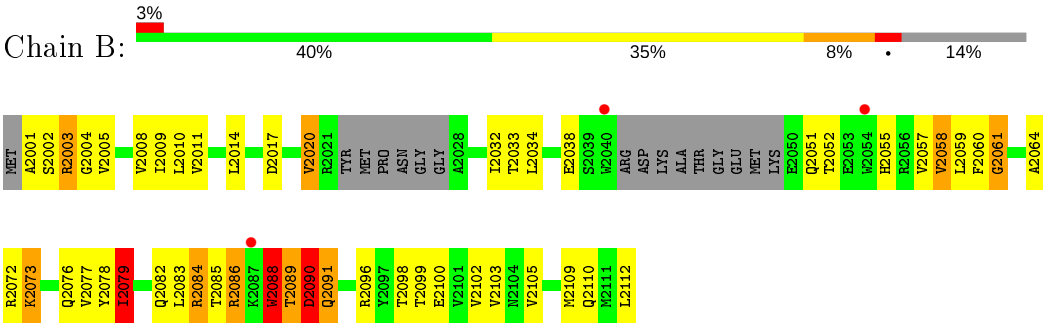
- Molecule 1: Single-strand binding protein

Chain A:



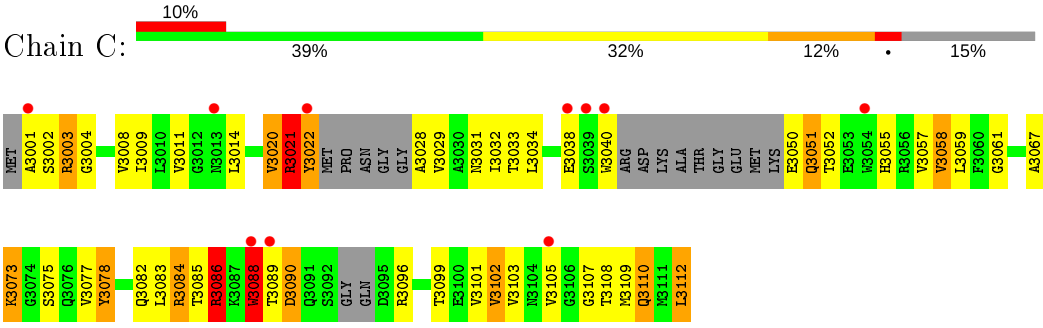
- Molecule 1: Single-strand binding protein

Chain B:



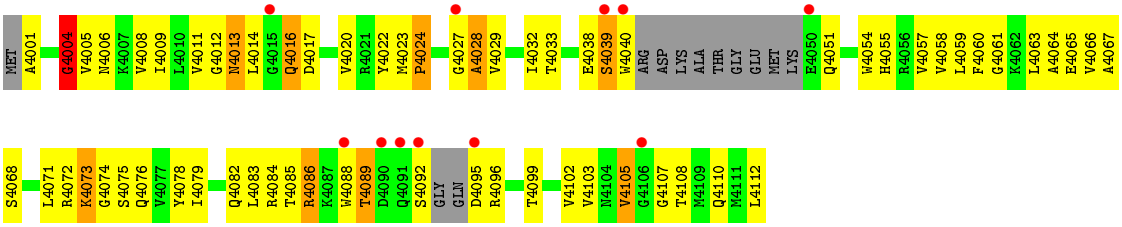
- Molecule 1: Single-strand binding protein

Chain C:



- Molecule 1: Single-strand binding protein

Chain D:


MET A4001
G4004 V4005 N4006 K4007 V4008 I4009 L4010 V4011 G4012 N4013 L4014 G4015 Q4016 D4017
V4020 R4021 Y4022 M4023 P4024
G4027 A4028 V4029
I4032 T4033
E4038 S4039 W4040
ARG ASP LYS ALA THR GLY GLU MET LYS
E4050 Q4051
W4054 H4055 R4056 V4057 V4058 L4059 F4060 G4061 K4062 L4063 A4064 E4065 V4066 A4067
S4068 L4071 R4072 K4073 G4074 S4075 Q4076 V4077 Y4078 I4079
Q4082 L4083 R4084 T4085 R4086 K4087 W4088 T4089 D4090 Q4091 S4092
GLY GLN D4095 R4096
T4099
V4102 V4103 W4104 V4105 G4106 G4107 T4108 M4109 Q4110 M4111 L4112

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	60.85Å 60.85Å 348.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 3.30 19.92 – 3.29	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.92-3.30) 97.8 (19.92-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.26 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.288 , 0.309 0.286 , 0.301	Depositor DCC
R_{free} test set	1196 reflections (10.34%)	wwPDB-VP
Wilson B-factor (Å^2)	106.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 118.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.075 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	2808	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.76	0/707	0.88	0/966
1	B	1.57	12/696 (1.7%)	1.48	15/950 (1.6%)
1	C	1.65	13/707 (1.8%)	1.42	12/963 (1.2%)
1	D	0.82	0/733	0.93	3/999 (0.3%)
All	All	1.26	25/2843 (0.9%)	1.21	30/3878 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2088	TRP	CG-CD1	-16.84	1.13	1.36
1	C	3088	TRP	CG-CD1	-16.16	1.14	1.36
1	C	3058	VAL	CB-CG2	-14.08	1.23	1.52
1	C	3020	VAL	CB-CG2	-13.34	1.24	1.52
1	B	2058	VAL	CB-CG2	-12.11	1.27	1.52
1	B	2058	VAL	CB-CG1	-11.64	1.28	1.52
1	C	3058	VAL	CB-CG1	-10.53	1.30	1.52
1	C	3052	THR	CB-CG2	-10.01	1.19	1.52
1	B	2052	THR	CB-CG2	-9.93	1.19	1.52
1	B	2071	LEU	CG-CD1	-9.81	1.15	1.51
1	B	2020	VAL	CB-CG2	-9.37	1.33	1.52
1	B	2020	VAL	CB-CG1	-9.22	1.33	1.52
1	C	3071	LEU	CG-CD1	-8.80	1.19	1.51
1	C	3020	VAL	CB-CG1	-8.57	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3071	LEU	CG-CD2	-8.09	1.22	1.51
1	B	2071	LEU	CG-CD2	-7.59	1.23	1.51
1	B	2088	TRP	CB-CG	-6.97	1.37	1.50
1	C	3088	TRP	CD2-CE3	-6.56	1.30	1.40
1	B	2089	THR	C-O	-6.45	1.11	1.23
1	C	3088	TRP	NE1-CE2	-6.03	1.29	1.37
1	C	3089	THR	C-O	-5.90	1.12	1.23
1	B	2088	TRP	CE3-CZ3	-5.78	1.28	1.38
1	C	3088	TRP	CB-CG	-5.75	1.39	1.50
1	B	2088	TRP	CD2-CE3	-5.40	1.32	1.40
1	C	3088	TRP	CE3-CZ3	-5.32	1.29	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2086	ARG	NE-CZ-NH2	12.02	126.31	120.30
1	C	3058	VAL	CG1-CB-CG2	-11.69	92.20	110.90
1	C	3071	LEU	CD1-CG-CD2	-11.09	77.22	110.50
1	B	2071	LEU	CD1-CG-CD2	-10.92	77.74	110.50
1	C	3020	VAL	CG1-CB-CG2	-10.79	93.63	110.90
1	B	2020	VAL	CG1-CB-CG2	-10.79	93.64	110.90
1	B	2058	VAL	CG1-CB-CG2	-10.60	93.95	110.90
1	B	2052	THR	OG1-CB-CG2	-10.05	86.89	110.00
1	C	3052	THR	OG1-CB-CG2	-8.91	89.51	110.00
1	B	2084	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	2086	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	C	3084	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	B	2090	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	B	2079	ILE	CG1-CB-CG2	-7.65	94.56	111.40
1	C	3021	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	3086	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	C	3084	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	B	2088	TRP	CB-CG-CD2	6.64	135.24	126.60
1	B	2088	TRP	CB-CG-CD1	-6.50	118.55	127.00
1	B	2084	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	2089	THR	CA-C-N	6.34	131.16	117.20
1	C	3088	TRP	CB-CG-CD2	6.21	134.67	126.60
1	C	3088	TRP	CB-CG-CD1	-6.00	119.19	127.00
1	C	3089	THR	CA-C-N	5.97	130.33	117.20
1	D	4086	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	B	2088	TRP	CG-CD1-NE1	5.69	115.79	110.10
1	C	3090	ASP	CB-CG-OD2	-5.62	113.24	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4063	LEU	CA-CB-CG	5.16	127.18	115.30
1	D	4004	GLY	N-CA-C	5.13	125.92	113.10
1	B	2071	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Sidechain
1	C	3078	TYR	Sidechain

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	698	0	632	52	0
1	B	688	0	628	54	0
1	C	698	0	635	64	0
1	D	724	0	661	77	0
All	All	2808	0	2556	207	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 39.

All (207) 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:2089:THR:O	1:B:2090:ASP:HB3	1.53	1.09
1:D:4020:VAL:HG21	1:D:4068:SER:HB2	1.37	1.06
1:C:3014:LEU:HD23	1:C:3034:LEU:HD23	1.42	0.97
1:C:3077:VAL:HG23	1:C:3110:GLN:O	1.63	0.97
1:C:3011:VAL:O	1:D:4004:GLY:HA3	1.63	0.97
1:A:1020:VAL:HG21	1:A:1068:SER:HB2	1.49	0.93
1:D:4084:ARG:HH21	1:D:4086:ARG:HD2	1.34	0.92
1:B:2088:TRP:CD1	1:B:2088:TRP:C	2.44	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3096:ARG:HH11	1:D:4096:ARG:NH1	1.70	0.88
1:C:3096:ARG:NH1	1:D:4096:ARG:HH11	1.71	0.87
1:C:3084:ARG:HH21	1:C:3086:ARG:HD3	1.38	0.87
1:A:1089:THR:HG22	1:A:1095:ASP:OD1	1.74	0.86
1:A:1012:GLY:C	1:A:1013:ASN:HD22	1.78	0.85
1:A:1023:MET:HB2	1:A:1024:PRO:HD2	1.57	0.84
1:C:3001:ALA:HA	1:D:4039:SER:H	1.41	0.84
1:B:2077:VAL:HG23	1:B:2110:GLN:O	1.79	0.83
1:D:4084:ARG:HH21	1:D:4086:ARG:CD	1.93	0.82
1:C:3096:ARG:HD3	1:D:4096:ARG:HH12	1.45	0.81
1:C:3088:TRP:HD1	1:C:3088:TRP:N	1.79	0.80
1:D:4020:VAL:HG21	1:D:4068:SER:CB	2.12	0.80
1:C:3086:ARG:HH11	1:C:3086:ARG:CG	1.94	0.79
1:C:3032:ILE:HG13	1:C:3057:VAL:HB	1.65	0.78
1:C:3086:ARG:HG2	1:C:3086:ARG:HH11	1.48	0.78
1:C:3096:ARG:HH11	1:D:4096:ARG:HH11	0.85	0.76
1:C:3099:THR:HB	1:D:4099:THR:HG21	1.68	0.76
1:D:4084:ARG:NH2	1:D:4086:ARG:HD2	2.00	0.75
1:A:1022:TYR:HB3	1:A:1027:GLY:HA3	1.68	0.75
1:C:3050:GLU:HG2	1:C:3051:GLN:H	1.52	0.74
1:A:1032:ILE:HG13	1:A:1057:VAL:HB	1.68	0.74
1:B:2088:TRP:HD1	1:B:2088:TRP:C	1.90	0.73
1:C:3096:ARG:HD3	1:D:4096:ARG:NH1	2.03	0.73
1:A:1001:ALA:HA	1:B:2038:GLU:HA	1.69	0.73
1:C:3088:TRP:CD1	1:C:3088:TRP:N	2.54	0.72
1:D:4066:VAL:HG13	1:D:4067:ALA:N	2.06	0.70
1:C:3014:LEU:HD23	1:C:3034:LEU:CD2	2.20	0.70
1:C:3096:ARG:CD	1:D:4096:ARG:NH1	2.55	0.70
1:B:2002:SER:HA	1:D:4110:GLN:NE2	2.06	0.69
1:B:2089:THR:O	1:B:2090:ASP:CB	2.26	0.69
1:C:3050:GLU:HG2	1:C:3051:GLN:N	2.06	0.69
1:B:2034:LEU:HD11	1:B:2079:ILE:HD13	1.74	0.68
1:D:4022:TYR:HB3	1:D:4027:GLY:HA3	1.76	0.68
1:C:3088:TRP:HD1	1:C:3088:TRP:H	1.44	0.66
1:A:1013:ASN:HD22	1:A:1013:ASN:N	1.91	0.66
1:A:1039:SER:H	1:B:2001:ALA:HA	1.60	0.66
1:C:3011:VAL:HB	1:D:4005:VAL:H	1.61	0.66
1:B:2014:LEU:HB2	1:B:2073:LYS:O	1.95	0.66
1:A:1014:LEU:HD11	1:A:1071:LEU:HD23	1.78	0.65
1:D:4057:VAL:HG11	1:D:4079:ILE:HD13	1.78	0.65
1:A:1039:SER:O	1:A:1040:TRP:HB3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4039:SER:O	1:D:4040:TRP:HB3	1.96	0.64
1:A:1096:ARG:HG2	1:B:2096:ARG:HH12	1.62	0.64
1:B:2088:TRP:HD1	1:B:2089:THR:N	1.95	0.64
1:A:1023:MET:O	1:A:1024:PRO:O	2.16	0.63
1:C:3096:ARG:CD	1:D:4096:ARG:HH12	2.09	0.63
1:C:3014:LEU:HB2	1:C:3073:LYS:O	1.98	0.63
1:C:3038:GLU:HA	1:D:4001:ALA:HA	1.78	0.63
1:C:3084:ARG:NH2	1:C:3086:ARG:HD3	2.12	0.63
1:A:1014:LEU:HD22	1:A:1032:ILE:HB	1.80	0.62
1:B:2076:GLN:HG2	1:B:2112:LEU:HD12	1.82	0.61
1:C:3099:THR:HB	1:D:4099:THR:CG2	2.30	0.61
1:A:1090:ASP:CG	1:A:1091:GLN:H	2.02	0.61
1:D:4006:ASN:ND2	1:D:4082:GLN:HB3	2.16	0.61
1:A:1090:ASP:OD1	1:A:1091:GLN:N	2.25	0.60
1:A:1008:VAL:HA	1:B:2008:VAL:HA	1.84	0.59
1:D:4040:TRP:CD1	1:D:4040:TRP:O	2.55	0.59
1:A:1108:THR:HG22	1:A:1109:MET:N	2.18	0.59
1:A:1005:VAL:O	1:B:2010:LEU:HA	2.04	0.58
1:B:2090:ASP:OD1	1:B:2090:ASP:C	2.42	0.58
1:A:1020:VAL:HG21	1:A:1068:SER:CB	2.30	0.58
1:C:3001:ALA:CA	1:D:4039:SER:H	2.13	0.57
1:C:3090:ASP:C	1:C:3090:ASP:OD1	2.43	0.57
1:C:3050:GLU:CG	1:C:3051:GLN:H	2.16	0.57
1:D:4085:THR:HA	1:D:4099:THR:HA	1.86	0.56
1:C:3001:ALA:HA	1:D:4038:GLU:HA	1.87	0.56
1:D:4072:ARG:O	1:D:4073:LYS:C	2.44	0.56
1:D:4006:ASN:HD21	1:D:4082:GLN:HB3	1.71	0.56
1:B:2032:ILE:HG13	1:B:2057:VAL:HB	1.87	0.56
1:C:3002:SER:O	1:C:3003:ARG:O	2.23	0.56
1:C:3031:ASN:OD1	1:C:3058:VAL:HG23	2.05	0.56
1:B:2002:SER:HA	1:D:4110:GLN:HE22	1.69	0.55
1:A:1066:VAL:HG13	1:A:1067:ALA:N	2.22	0.55
1:B:2014:LEU:HD22	1:B:2032:ILE:HB	1.89	0.55
1:C:3008:VAL:HA	1:D:4008:VAL:HA	1.88	0.55
1:A:1065:GLU:O	1:A:1068:SER:HB3	2.06	0.55
1:B:2002:SER:O	1:B:2003:ARG:O	2.24	0.55
1:B:2084:ARG:NH2	1:B:2100:GLU:OE2	2.40	0.55
1:C:3022:TYR:N	1:C:3022:TYR:CD2	2.75	0.54
1:A:1014:LEU:HB2	1:A:1073:LYS:O	2.08	0.54
1:B:2059:LEU:HD23	1:B:2103:VAL:HB	1.88	0.54
1:A:1053:GLU:OE1	1:B:2084:ARG:HA	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LEU:HD12	1:A:1109:MET:HB3	1.89	0.54
1:B:2060:PHE:HE1	1:B:2102:VAL:HG23	1.73	0.54
1:B:2058:VAL:HG12	1:B:2060:PHE:CE1	2.43	0.53
1:A:1085:THR:HG23	1:A:1099:THR:OG1	2.07	0.53
1:B:2020:VAL:HG21	1:B:2068:SER:HB2	1.89	0.53
1:A:1004:GLY:CA	1:B:2011:VAL:O	2.57	0.53
1:C:3002:SER:O	1:C:3003:ARG:C	2.48	0.52
1:C:3033:THR:HA	1:C:3055:HIS:O	2.10	0.51
1:A:1002:SER:O	1:A:1003:ARG:O	2.29	0.51
1:D:4066:VAL:CG1	1:D:4067:ALA:N	2.72	0.51
1:D:4089:THR:HG23	1:D:4095:ASP:OD1	2.10	0.51
1:A:1072:ARG:O	1:A:1073:LYS:C	2.48	0.51
1:C:3096:ARG:HD2	1:D:4096:ARG:NH1	2.25	0.51
1:C:3085:THR:HA	1:C:3099:THR:HA	1.93	0.51
1:D:4020:VAL:CG2	1:D:4068:SER:HB2	2.27	0.51
1:D:4033:THR:HG22	1:D:4054:TRP:HE3	1.76	0.51
1:D:4058:VAL:CG2	1:D:4102:VAL:HG12	2.41	0.50
1:D:4013:ASN:HA	1:D:4075:SER:O	2.10	0.50
1:A:1013:ASN:N	1:A:1013:ASN:ND2	2.59	0.50
1:A:1072:ARG:O	1:A:1073:LYS:O	2.29	0.50
1:B:2085:THR:HA	1:B:2099:THR:HA	1.94	0.50
1:D:4032:ILE:HG13	1:D:4057:VAL:HB	1.92	0.50
1:C:3028:ALA:O	1:C:3029:VAL:CG2	2.59	0.50
1:D:4032:ILE:HD11	1:D:4079:ILE:HD11	1.94	0.50
1:D:4064:ALA:O	1:D:4067:ALA:HB3	2.10	0.50
1:C:3077:VAL:CG2	1:C:3110:GLN:O	2.48	0.50
1:C:3021:ARG:C	1:C:3022:TYR:CD2	2.86	0.50
1:C:3004:GLY:HA2	1:D:4011:VAL:O	2.12	0.50
1:D:4023:MET:HB2	1:D:4024:PRO:HD2	1.93	0.50
1:D:4033:THR:HA	1:D:4055:HIS:O	2.11	0.49
1:A:1083:LEU:HD11	1:B:2083:LEU:HD21	1.93	0.49
1:A:1112:LEU:HD13	1:D:4112:LEU:HD13	1.93	0.49
1:D:4032:ILE:CG1	1:D:4057:VAL:HB	2.42	0.49
1:A:1032:ILE:CG1	1:A:1057:VAL:HB	2.39	0.49
1:A:1067:ALA:HA	1:A:1071:LEU:HD13	1.95	0.48
1:B:2002:SER:O	1:B:2003:ARG:C	2.51	0.48
1:A:1010:LEU:HA	1:B:2005:VAL:O	2.13	0.48
1:B:2077:VAL:HG21	1:B:2109:MET:HG2	1.94	0.48
1:C:3103:VAL:HG12	1:C:3103:VAL:O	2.12	0.48
1:C:3086:ARG:CG	1:C:3086:ARG:NH1	2.63	0.48
1:B:2033:THR:HA	1:B:2055:HIS:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2034:LEU:CD1	1:B:2079:ILE:HD13	2.43	0.47
1:C:3102:VAL:O	1:C:3102:VAL:CG2	2.61	0.47
1:D:4065:GLU:O	1:D:4068:SER:HB3	2.14	0.47
1:A:1008:VAL:CG1	1:A:1101:VAL:HG13	2.43	0.47
1:C:3001:ALA:HA	1:D:4039:SER:N	2.19	0.47
1:D:4022:TYR:HB3	1:D:4027:GLY:CA	2.44	0.47
1:A:1061:GLY:O	1:A:1064:ALA:HB3	2.14	0.47
1:C:3077:VAL:HG22	1:C:3078:TYR:N	2.30	0.47
1:D:4073:LYS:O	1:D:4075:SER:N	2.47	0.47
1:B:2077:VAL:HG22	1:B:2078:TYR:N	2.29	0.47
1:C:3021:ARG:NH2	1:C:3022:TYR:C	2.68	0.47
1:C:3077:VAL:HG21	1:C:3109:MET:HG2	1.95	0.47
1:A:1083:LEU:HD21	1:B:2083:LEU:HD11	1.97	0.47
1:C:3059:LEU:HD23	1:C:3103:VAL:HB	1.97	0.47
1:D:4089:THR:CG2	1:D:4095:ASP:OD1	2.64	0.46
1:D:4107:GLY:O	1:D:4108:THR:CG2	2.64	0.46
1:A:1060:PHE:O	1:A:1061:GLY:C	2.52	0.46
1:A:1066:VAL:O	1:A:1067:ALA:C	2.54	0.46
1:D:4023:MET:HB2	1:D:4024:PRO:CD	2.45	0.46
1:D:4066:VAL:HG13	1:D:4067:ALA:H	1.81	0.46
1:C:3083:LEU:HD11	1:D:4083:LEU:HD11	1.98	0.46
1:D:4085:THR:OG1	1:D:4099:THR:HB	2.15	0.46
1:A:1108:THR:CG2	1:A:1109:MET:N	2.78	0.46
1:D:4009:ILE:HG23	1:D:4078:TYR:CE1	2.51	0.46
1:B:2072:ARG:O	1:B:2073:LYS:C	2.55	0.45
1:C:3107:GLY:O	1:C:3108:THR:HB	2.16	0.45
1:C:3008:VAL:HG11	1:C:3101:VAL:HG13	1.98	0.45
1:D:4016:GLN:HG2	1:D:4017:ASP:O	2.16	0.45
1:C:3077:VAL:HG23	1:C:3110:GLN:C	2.34	0.45
1:B:2086:ARG:HD2	1:B:2086:ARG:HH11	1.56	0.45
1:A:1066:VAL:HG13	1:A:1067:ALA:H	1.81	0.44
1:D:4028:ALA:C	1:D:4029:VAL:HG23	2.37	0.44
1:D:4014:LEU:HB2	1:D:4073:LYS:O	2.17	0.44
1:C:3040:TRP:CD1	1:C:3040:TRP:N	2.85	0.44
1:D:4060:PHE:O	1:D:4061:GLY:C	2.56	0.44
1:A:1008:VAL:HG11	1:A:1101:VAL:HG13	1.99	0.44
1:B:2059:LEU:HD21	1:B:2103:VAL:HG21	2.00	0.44
1:D:4032:ILE:HD11	1:D:4079:ILE:CD1	2.47	0.44
1:A:1085:THR:HA	1:A:1099:THR:HA	1.99	0.43
1:B:2102:VAL:O	1:B:2102:VAL:HG13	2.19	0.43
1:B:2059:LEU:CD2	1:B:2103:VAL:HG21	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3102:VAL:HG23	1:C:3102:VAL:O	2.19	0.43
1:D:4059:LEU:HD23	1:D:4103:VAL:CG2	2.49	0.43
1:D:4014:LEU:HD12	1:D:4014:LEU:N	2.33	0.43
1:D:4065:GLU:OE2	1:D:4065:GLU:HA	2.18	0.43
1:D:4107:GLY:C	1:D:4108:THR:HG23	2.39	0.43
1:D:4027:GLY:O	1:D:4028:ALA:HB2	2.19	0.43
1:D:4105:VAL:C	1:D:4107:GLY:H	2.22	0.43
1:B:2032:ILE:CG1	1:B:2057:VAL:HB	2.47	0.43
1:A:1011:VAL:O	1:B:2004:GLY:CA	2.67	0.43
1:D:4028:ALA:O	1:D:4029:VAL:CG2	2.66	0.43
1:A:1014:LEU:CD2	1:A:1032:ILE:HB	2.47	0.42
1:B:2088:TRP:HE1	1:B:2090:ASP:HB2	1.84	0.42
1:B:2103:VAL:HG12	1:B:2103:VAL:O	2.19	0.42
1:B:2009:ILE:HD13	1:C:3009:ILE:HD13	2.01	0.42
1:B:2008:VAL:HG13	1:B:2008:VAL:O	2.19	0.42
1:C:3067:ALA:O	1:C:3071:LEU:HB2	2.20	0.42
1:D:4058:VAL:HG23	1:D:4058:VAL:O	2.18	0.42
1:D:4012:GLY:O	1:D:4076:GLN:HA	2.19	0.42
1:A:1006:ASN:C	1:A:1006:ASN:OD1	2.57	0.42
1:D:4023:MET:O	1:D:4024:PRO:O	2.38	0.42
1:C:3112:LEU:CD1	1:C:3112:LEU:N	2.82	0.41
1:D:4059:LEU:CD2	1:D:4103:VAL:HG21	2.50	0.41
1:C:3099:THR:CB	1:D:4099:THR:HG21	2.45	0.41
1:A:1004:GLY:HA2	1:B:2011:VAL:O	2.20	0.41
1:B:2088:TRP:HZ3	1:B:2098:THR:HG1	1.69	0.41
1:B:2091:GLN:HG3	1:B:2091:GLN:H	1.53	0.41
1:A:1011:VAL:HB	1:B:2005:VAL:H	1.85	0.41
1:D:4067:ALA:O	1:D:4071:LEU:HB2	2.20	0.41
1:A:1022:TYR:CD2	1:A:1027:GLY:O	2.74	0.41
1:B:2077:VAL:CG2	1:B:2109:MET:HG2	2.50	0.41
1:C:3032:ILE:CG1	1:C:3057:VAL:HB	2.44	0.41
1:B:2061:GLY:O	1:B:2064:ALA:HB3	2.21	0.41
1:C:3055:HIS:HD2	1:D:4083:LEU:HD23	1.86	0.41
1:A:1011:VAL:O	1:B:2004:GLY:HA2	2.21	0.40
1:C:3014:LEU:HD22	1:C:3032:ILE:HB	2.03	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	94/113 (83%)	77 (82%)	9 (10%)	8 (8%)	1	5
1	B	91/113 (80%)	78 (86%)	6 (7%)	7 (8%)	1	6
1	C	88/113 (78%)	74 (84%)	8 (9%)	6 (7%)	1	8
1	D	95/113 (84%)	78 (82%)	10 (10%)	7 (7%)	1	7
All	All	368/452 (81%)	307 (83%)	33 (9%)	28 (8%)	1	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1003	ARG
1	A	1024	PRO
1	A	1073	LYS
1	A	1105	VAL
1	B	2051	GLN
1	B	2105	VAL
1	C	3105	VAL
1	D	4024	PRO
1	D	4073	LYS
1	D	4105	VAL
1	A	1004	GLY
1	B	2003	ARG
1	B	2061	GLY
1	B	2091	GLN
1	C	3003	ARG
1	C	3051	GLN
1	C	3061	GLY
1	D	4004	GLY
1	D	4074	GLY
1	A	1061	GLY
1	B	2073	LYS
1	D	4028	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1074	GLY
1	B	2090	ASP
1	C	3073	LYS
1	D	4016	GLN
1	A	1017	ASP
1	C	3075	SER

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	63/94 (67%)	59 (94%)	4 (6%)	18 47
1	B	64/94 (68%)	60 (94%)	4 (6%)	18 47
1	C	64/94 (68%)	55 (86%)	9 (14%)	3 16
1	D	69/94 (73%)	63 (91%)	6 (9%)	10 34
All	All	260/376 (69%)	237 (91%)	23 (9%)	10 33

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

Mol	Chain	Res	Type
1	A	1013	ASN
1	A	1021	ARG
1	A	1031	ASN
1	A	1059	LEU
1	B	2017	ASP
1	B	2079	ILE
1	B	2082	GLN
1	B	2088	TRP
1	C	3020	VAL
1	C	3021	ARG
1	C	3022	TYR
1	C	3082	GLN
1	C	3086	ARG
1	C	3088	TRP
1	C	3102	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3110	GLN
1	C	3112	LEU
1	D	4013	ASN
1	D	4039	SER
1	D	4051	GLN
1	D	4088	TRP
1	D	4089	THR
1	D	4092	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1013	ASN
1	A	1031	ASN
1	A	1076	GLN
1	B	2051	GLN
1	B	2110	GLN
1	C	3055	HIS
1	C	3110	GLN
1	D	4016	GLN
1	D	4031	ASN
1	D	4051	GLN
1	D	4110	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

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^{th} 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	100/113 (88%)	0.24	9 (9%) 9 9	49, 97, 168, 200	0
1	B	97/113 (85%)	0.06	3 (3%) 49 48	51, 99, 164, 192	0
1	C	96/113 (84%)	0.28	11 (11%) 4 4	50, 106, 173, 200	0
1	D	101/113 (89%)	0.30	11 (10%) 5 5	38, 92, 169, 200	0
All	All	394/452 (87%)	0.22	34 (8%) 10 10	38, 98, 169, 200	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4095	ASP	5.9
1	A	1095	ASP	5.4
1	A	1096	ARG	4.6
1	C	3039	SER	4.5
1	A	1088	TRP	4.2
1	D	4092	SER	3.9
1	A	1050	GLU	3.6
1	D	4039	SER	3.5
1	A	1039	SER	3.4
1	C	3001	ALA	3.2
1	A	1089	THR	3.1
1	D	4015	GLY	3.0
1	C	3022	TYR	2.9
1	B	2040	TRP	2.9
1	D	4027	GLY	2.7
1	D	4040	TRP	2.7
1	D	4090	ASP	2.6
1	C	3088	TRP	2.6
1	D	4050	GLU	2.6
1	C	3040	TRP	2.5
1	C	3013	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	4091	GLN	2.4
1	C	3038	GLU	2.4
1	D	4088	TRP	2.4
1	C	3068	SER	2.4
1	A	1027	GLY	2.4
1	C	3089	THR	2.4
1	A	1001	ALA	2.3
1	B	2054	TRP	2.3
1	C	3054	TRP	2.2
1	A	1090	ASP	2.2
1	B	2087	LYS	2.2
1	C	3105	VAL	2.2
1	D	4106	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.