Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:10 PM GMT

PDB ID	:	1SG2
Title	:	Crystal structure of the periplasmic chaperone Skp
Authors	:	Korndorfer, I.P.; Dommel, M.K.; Skerra, A.
Deposited on	:	2004-02-23
Resolution	:	2.35 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
http://wwpdb.org/validation/2016/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:

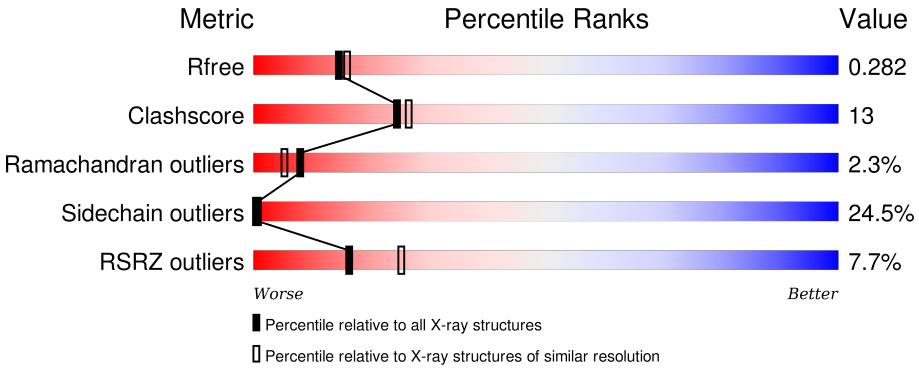
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	153	10%, 46%, 33%, 10%, 8%
1	B	153	6%, 39%, 22%, 9%, 29%
1	C	153	4%, 58%, 29%, 7%, 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3119 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 Seventeen Kilodalton Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1097	668	204	220	5			
1	B	109	Total	C	N	O	S	0	0	0
			834	507	156	169	2			
1	C	142	Total	C	N	O	S	0	0	0
			1102	671	205	221	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	STREP-TAGII	UNP P0AEU7
A	2	SER	-	STREP-TAGII	UNP P0AEU7
A	3	TRP	-	STREP-TAGII	UNP P0AEU7
A	4	SER	-	STREP-TAGII	UNP P0AEU7
A	5	HIS	-	STREP-TAGII	UNP P0AEU7
A	6	PRO	-	STREP-TAGII	UNP P0AEU7
A	7	GLN	-	STREP-TAGII	UNP P0AEU7
A	8	PHE	-	STREP-TAGII	UNP P0AEU7
A	9	GLU	-	STREP-TAGII	UNP P0AEU7
A	10	LYS	-	STREP-TAGII	UNP P0AEU7
A	11	GLY	-	LINKER	UNP P0AEU7
A	11	GLY	-	LINKER	UNP P0AEU7
B	1	ALA	-	STREP-TAGII	UNP P0AEU7
B	2	SER	-	STREP-TAGII	UNP P0AEU7
B	3	TRP	-	STREP-TAGII	UNP P0AEU7
B	4	SER	-	STREP-TAGII	UNP P0AEU7
B	5	HIS	-	STREP-TAGII	UNP P0AEU7
B	6	PRO	-	STREP-TAGII	UNP P0AEU7
B	7	GLN	-	STREP-TAGII	UNP P0AEU7
B	8	PHE	-	STREP-TAGII	UNP P0AEU7
B	9	GLU	-	STREP-TAGII	UNP P0AEU7
B	10	LYS	-	STREP-TAGII	UNP P0AEU7
B	11	GLY	-	LINKER	UNP P0AEU7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	GLY	-	LINKER	UNP P0AEU7
C	1	ALA	-	STREP-TAGII	UNP P0AEU7
C	2	SER	-	STREP-TAGII	UNP P0AEU7
C	3	TRP	-	STREP-TAGII	UNP P0AEU7
C	4	SER	-	STREP-TAGII	UNP P0AEU7
C	5	HIS	-	STREP-TAGII	UNP P0AEU7
C	6	PRO	-	STREP-TAGII	UNP P0AEU7
C	7	GLN	-	STREP-TAGII	UNP P0AEU7
C	8	PHE	-	STREP-TAGII	UNP P0AEU7
C	9	GLU	-	STREP-TAGII	UNP P0AEU7
C	10	LYS	-	STREP-TAGII	UNP P0AEU7
C	11	GLY	-	LINKER	UNP P0AEU7
C	11	GLY	-	LINKER	UNP P0AEU7

- Molecule 2 is water.

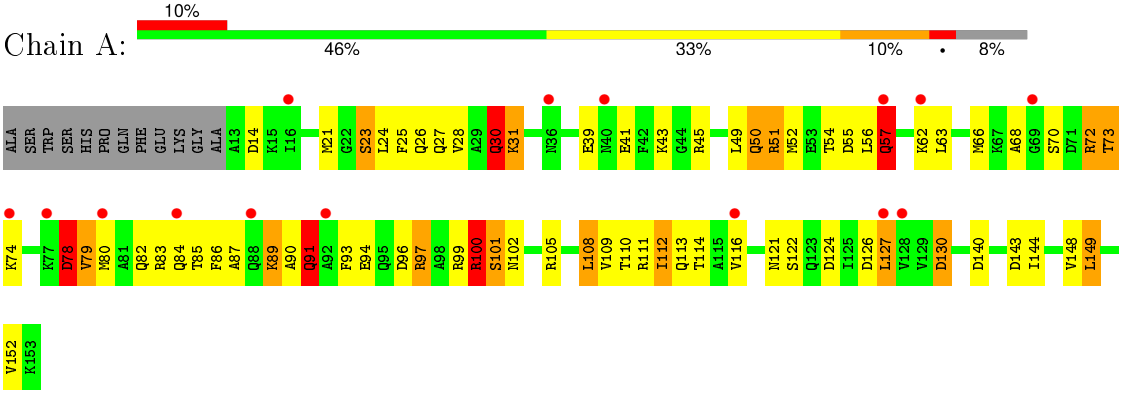
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	28	Total O 28 28	0	0
2	B	28	Total O 28 28	0	0
2	C	30	Total O 30 30	0	0

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.

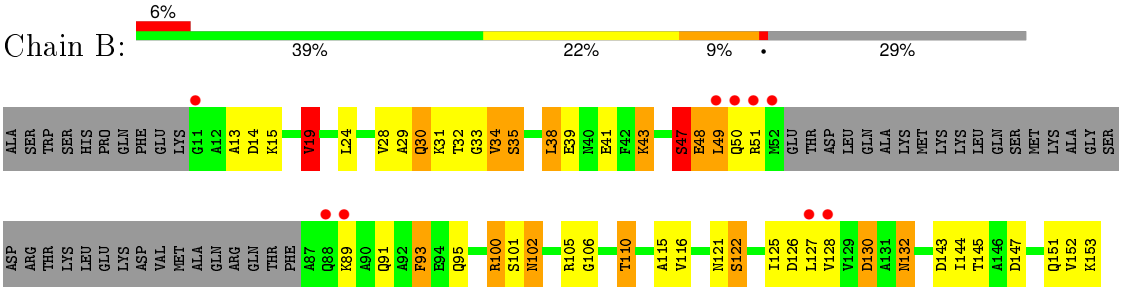
- Molecule 1: Seventeen Kilodalton Protein

Chain A:



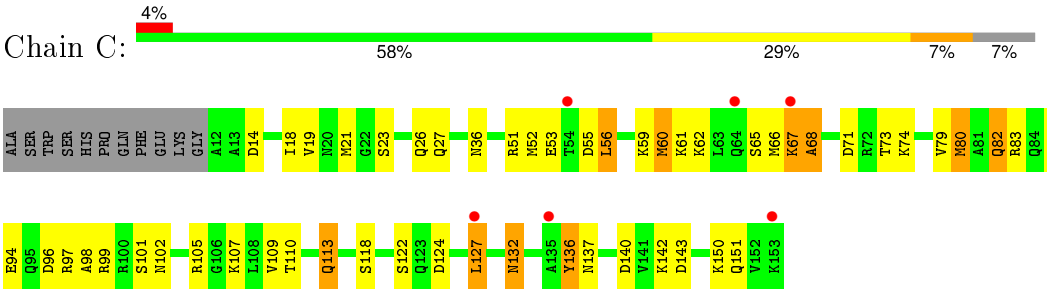
- Molecule 1: Seventeen Kilodalton Protein

Chain B:



- Molecule 1: Seventeen Kilodalton Protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.98Å 83.91Å 158.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 19.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.35) 93.4 (19.91-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.279 0.226 , 0.282	Depositor DCC
R_{free} test set	1439 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	6 of 35281 reflections (0.017%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3119	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.65	0/1101	1.48	17/1470 (1.2%)
1	B	0.77	0/836	1.49	15/1119 (1.3%)
1	C	0.78	2/1106 (0.2%)	1.45	16/1477 (1.1%)
All	All	0.73	2/3043 (0.1%)	1.47	48/4066 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	TYR	CD1-CE1	-5.63	1.30	1.39
1	C	21	MET	SD-CE	-5.45	1.47	1.77

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	124	ASP	CB-CG-OD2	11.38	128.54	118.30
1	B	126	ASP	CB-CG-OD2	11.04	128.23	118.30
1	A	14	ASP	CB-CG-OD2	10.65	127.89	118.30
1	A	124	ASP	CB-CG-OD1	10.48	127.73	118.30
1	A	126	ASP	CB-CG-OD1	-10.32	109.01	118.30
1	A	126	ASP	CB-CG-OD2	9.86	127.18	118.30
1	A	100	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	B	126	ASP	CB-CG-OD1	-9.30	109.93	118.30
1	B	147	ASP	CB-CG-OD2	9.19	126.58	118.30
1	B	19	VAL	CB-CA-C	-8.75	94.77	111.40
1	B	100	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	140	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	127	LEU	CB-CG-CD2	7.88	124.39	111.00
1	C	140	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	130	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	A	114	THR	OG1-CB-CG2	-7.45	92.87	110.00
1	A	143	ASP	CB-CG-OD2	7.31	124.88	118.30
1	C	143	ASP	CB-CG-OD1	6.77	124.40	118.30
1	A	55	ASP	CB-CG-OD2	6.65	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	124	ASP	OD1-CG-OD2	-6.65	110.67	123.30
1	A	100	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	C	127	LEU	CA-CB-CG	6.58	130.43	115.30
1	C	21	MET	CG-SD-CE	-6.58	89.68	100.20
1	A	127	LEU	CB-CA-C	-6.49	97.86	110.20
1	A	149	LEU	CA-CB-CG	6.33	129.86	115.30
1	B	34	VAL	CB-CA-C	-6.31	99.41	111.40
1	B	147	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	78	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	145	THR	OG1-CB-CG2	-6.06	96.06	110.00
1	A	112	ILE	CG1-CB-CG2	-6.02	98.16	111.40
1	C	124	ASP	CB-CA-C	6.01	122.42	110.40
1	C	132	ASN	N-CA-CB	-5.97	99.85	110.60
1	B	122	SER	CA-CB-OG	-5.77	95.61	111.20
1	C	136	TYR	CB-CA-C	-5.68	99.05	110.40
1	C	151	GLN	N-CA-CB	-5.59	100.53	110.60
1	A	96	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	19	VAL	N-CA-CB	5.43	123.46	111.50
1	B	100	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	142	LYS	CD-CE-NZ	-5.34	99.41	111.70
1	C	51	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	99	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	19	VAL	CA-CB-CG2	5.20	118.69	110.90
1	B	51	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	121	ASN	CB-CA-C	-5.12	100.16	110.40
1	C	71	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	19	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	B	143	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	14	ASP	CB-CG-OD2	5.05	122.84	118.30

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	1097	0	1124	39	0
1	B	834	0	844	23	0
1	C	1102	0	1129	18	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	30	0	0	1	0
All	All	3119	0	3097	79	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 13.

All (79) 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:108:LEU:HD12	1:A:108:LEU:C	2.02	0.80
1:C:113:GLN:HE21	1:C:113:GLN:HA	1.46	0.79
1:A:63:LEU:HD22	1:A:72:ARG:HH11	1.50	0.76
1:A:24:LEU:O	1:A:28:VAL:HG13	1.88	0.73
1:A:86:PHE:O	1:A:86:PHE:CD2	2.43	0.72
1:A:86:PHE:HD2	1:A:86:PHE:O	1.76	0.69
1:B:24:LEU:O	1:B:28:VAL:HG23	1.92	0.69
1:A:63:LEU:HD22	1:A:72:ARG:NH1	2.08	0.68
1:A:41:GLU:OE2	1:A:100:ARG:NE	2.27	0.67
1:A:97:ARG:O	1:A:101:SER:HB2	1.95	0.66
1:A:23:SER:O	1:A:27:GLN:NE2	2.30	0.65
1:C:59:LYS:NZ	1:C:82:GLN:HE22	1.97	0.62
1:C:59:LYS:HZ3	1:C:82:GLN:HE22	1.47	0.62
1:B:130:ASP:OD2	1:B:132:ASN:ND2	2.33	0.61
1:B:102:ASN:O	1:B:105:ARG:HB3	2.02	0.60
1:C:56:LEU:HD21	1:C:82:GLN:HB3	1.85	0.59
1:B:19:VAL:HG22	1:B:128:VAL:HG12	1.84	0.59
1:B:93:PHE:C	1:B:93:PHE:CD2	2.75	0.59
1:C:62:LYS:O	1:C:66:MET:HG3	2.02	0.59
1:A:90:ALA:O	1:A:91:GLN:HB3	2.03	0.58
1:A:108:LEU:C	1:A:108:LEU:CD1	2.70	0.58
1:A:49:LEU:HD21	1:A:89:LYS:HB3	1.85	0.58
1:C:150:LYS:HG3	2:C:169:HOH:O	2.04	0.58
1:B:130:ASP:HB3	1:B:132:ASN:ND2	2.22	0.55
1:B:38:LEU:HD21	1:B:101:SER:HA	1.88	0.55
1:A:56:LEU:O	1:A:57:GLN:C	2.45	0.53
1:B:43:LYS:O	1:B:47:SER:HB2	2.08	0.53
1:B:19:VAL:HG22	1:B:128:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:CE1	1:A:108:LEU:HD11	2.43	0.53
1:B:132:ASN:HD22	1:B:132:ASN:H	1.55	0.53
1:C:52:MET:O	1:C:56:LEU:HB2	2.10	0.52
1:A:68:ALA:HA	1:C:73:THR:HG21	1.91	0.52
1:B:34:VAL:HG23	1:B:35:SER:N	2.25	0.51
1:C:98:ALA:O	1:C:102:ASN:HB2	2.11	0.51
1:B:41:GLU:OE2	1:B:100:ARG:HD3	2.10	0.51
1:B:115:ALA:O	1:B:116:VAL:C	2.48	0.51
1:A:50:GLN:O	1:A:51:ARG:C	2.49	0.50
1:A:144:ILE:O	1:A:148:VAL:HG23	2.10	0.50
1:B:28:VAL:O	1:B:32:THR:HG23	2.11	0.50
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.76	0.50
1:A:78:ASP:C	1:A:78:ASP:OD1	2.50	0.49
1:C:109:VAL:O	1:C:113:GLN:HG2	2.11	0.49
1:C:67:LYS:O	1:C:68:ALA:HB3	2.11	0.49
1:B:48:GLU:O	1:B:48:GLU:HG2	2.13	0.49
1:A:66:MET:HE2	1:A:72:ARG:HB2	1.96	0.48
1:A:54:THR:HA	1:A:57:GLN:HB2	1.95	0.48
1:A:85:THR:O	1:A:89:LYS:HB2	2.14	0.47
1:A:79:VAL:O	1:A:79:VAL:CG1	2.62	0.47
1:A:30:GLN:O	1:A:31:LYS:C	2.51	0.47
1:A:25:PHE:CE1	1:A:105:ARG:HG3	2.50	0.46
1:A:110:THR:O	1:A:111:ARG:C	2.52	0.46
1:A:148:VAL:O	1:A:152:VAL:HG23	2.16	0.46
1:C:136:TYR:CG	1:C:137:ASN:N	2.84	0.46
1:A:41:GLU:OE2	1:A:100:ARG:HD3	2.16	0.45
1:A:93:PHE:C	1:A:93:PHE:CD1	2.89	0.45
1:A:41:GLU:OE2	1:A:100:ARG:CD	2.65	0.45
1:B:151:GLN:O	1:B:152:VAL:C	2.53	0.45
1:B:19:VAL:HG13	1:B:144:ILE:HG13	1.97	0.45
1:A:70:SER:HA	1:A:73:THR:HB	1.99	0.45
1:A:56:LEU:HD11	1:A:82:GLN:HB3	1.99	0.45
1:C:18:ILE:HD13	1:C:18:ILE:HG21	1.77	0.44
1:A:112:ILE:O	1:A:116:VAL:HG23	2.18	0.44
1:A:25:PHE:CZ	1:A:105:ARG:HG3	2.53	0.44
1:A:144:ILE:HD13	1:A:144:ILE:HG21	1.80	0.44
1:C:56:LEU:CD2	1:C:82:GLN:HB3	2.47	0.43
1:A:121:ASN:O	1:A:122:SER:C	2.55	0.43
1:C:113:GLN:NE2	1:C:113:GLN:HA	2.26	0.43
1:C:23:SER:O	1:C:27:GLN:HG3	2.19	0.42
1:B:106:GLY:O	1:B:110:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:O	1:A:91:GLN:CB	2.67	0.42
1:C:60:MET:HE3	1:C:83:ARG:NH2	2.35	0.42
1:B:38:LEU:HD12	1:B:38:LEU:HA	1.83	0.41
1:B:13:ALA:O	1:B:14:ASP:C	2.57	0.41
1:A:79:VAL:HG13	1:A:79:VAL:O	2.21	0.41
1:B:29:ALA:O	1:B:30:GLN:C	2.58	0.41
1:B:33:GLY:O	1:B:34:VAL:C	2.58	0.40
1:C:79:VAL:O	1:C:80:MET:C	2.58	0.40
1:A:52:MET:HE2	1:A:52:MET:HB3	1.91	0.40
1:B:15:LYS:HE2	1:B:125:ILE:HG13	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	139/153 (91%)	122 (88%)	12 (9%)	5 (4%)	4 2
1	B	105/153 (69%)	91 (87%)	11 (10%)	3 (3%)	6 3
1	C	140/153 (92%)	136 (97%)	3 (2%)	1 (1%)	26 29
All	All	384/459 (84%)	349 (91%)	26 (7%)	9 (2%)	8 5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	B	47	SER
1	B	89	LYS
1	A	30	GLN
1	A	57	GLN
1	A	87	ALA
1	A	31	LYS

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Mol	Chain	Res	Type
1	B	49	LEU
1	C	68	ALA

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	119/128 (93%)	86 (72%)	33 (28%)	0	0
1	B	89/128 (70%)	68 (76%)	21 (24%)	1	0
1	C	119/128 (93%)	93 (78%)	26 (22%)	1	1
All	All	327/384 (85%)	247 (76%)	80 (24%)	1	0

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	23	SER
1	A	26	GLN
1	A	30	GLN
1	A	39	GLU
1	A	43	LYS
1	A	45	ARG
1	A	50	GLN
1	A	51	ARG
1	A	57	GLN
1	A	62	LYS
1	A	72	ARG
1	A	73	THR
1	A	74	LYS
1	A	78	ASP
1	A	79	VAL
1	A	80	MET
1	A	83	ARG
1	A	84	GLN
1	A	89	LYS

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	94	GLU
1	A	97	ARG
1	A	99	ARG
1	A	100	ARG
1	A	101	SER
1	A	102	ASN
1	A	108	LEU
1	A	109	VAL
1	A	113	GLN
1	A	127	LEU
1	A	130	ASP
1	A	149	LEU
1	B	19	VAL
1	B	30	GLN
1	B	31	LYS
1	B	35	SER
1	B	38	LEU
1	B	39	GLU
1	B	43	LYS
1	B	47	SER
1	B	48	GLU
1	B	49	LEU
1	B	50	GLN
1	B	91	GLN
1	B	93	PHE
1	B	95	GLN
1	B	102	ASN
1	B	110	THR
1	B	122	SER
1	B	127	LEU
1	B	130	ASP
1	B	132	ASN
1	B	153	LYS
1	C	26	GLN
1	C	36	ASN
1	C	53	GLU
1	C	55	ASP
1	C	56	LEU
1	C	60	MET
1	C	61	LYS
1	C	65	SER

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Mol	Chain	Res	Type
1	C	67	LYS
1	C	74	LYS
1	C	80	MET
1	C	82	GLN
1	C	85	THR
1	C	88	GLN
1	C	94	GLU
1	C	96	ASP
1	C	97	ARG
1	C	101	SER
1	C	105	ARG
1	C	107	LYS
1	C	110	THR
1	C	113	GLN
1	C	118	SER
1	C	122	SER
1	C	127	LEU
1	C	132	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	30	GLN
1	A	113	GLN
1	B	50	GLN
1	B	102	ASN
1	B	121	ASN
1	B	132	ASN
1	C	82	GLN
1	C	84	GLN
1	C	113	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	141/153 (92%)	0.51	15 (10%) 8 14	15, 57, 81, 99	0
1	B	109/153 (71%)	0.30	9 (8%) 14 22	14, 39, 91, 101	0
1	C	142/153 (92%)	0.25	6 (4%) 40 54	15, 45, 73, 80	0
All	All	392/459 (85%)	0.36	30 (7%) 16 25	14, 47, 82, 101	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	LYS	4.2
1	B	50	GLN	4.2
1	C	67	LYS	3.7
1	B	49	LEU	3.6
1	B	52	MET	3.2
1	B	127	LEU	3.2
1	A	57	GLN	3.1
1	C	64	GLN	3.0
1	A	128	VAL	2.9
1	A	88	GLN	2.9
1	B	128	VAL	2.8
1	B	89	LYS	2.8
1	A	62	LYS	2.7
1	C	54	THR	2.7
1	A	80	MET	2.7
1	B	51	ARG	2.7
1	C	127	LEU	2.6
1	A	69	GLY	2.6
1	B	11	GLY	2.5
1	B	88	GLN	2.5
1	A	40	ASN	2.4
1	A	74	LYS	2.3
1	A	84	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	92	ALA	2.3
1	A	36	ASN	2.2
1	A	16	ILE	2.2
1	C	153	LYS	2.2
1	A	116	VAL	2.2
1	C	135	ALA	2.1
1	A	127	LEU	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.