

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3F72
Title	:	Crystal Structure of the Staphylococcus aureus pI258 CadC Metal Binding
		Site 2 Mutant
Authors	:	Kandegedara, A.; Thiyagarajan, S.; Kondapalli, K.C.; Stemmler, T.L.; Rosen,
		B.P.
Deposited on	:	2008-11-07
Resolution	:	2.31 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolDuchitz		4 00h 467
MolProbity	:	4.020-407
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.31 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.



Matria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	5974(2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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 of 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%

Mol	Chain	Length	Quality of chain			
1	А	122	60%	25%	· •	12%
1	В	122	56%	23%	10%	11%
1	С	122	46%	30%	8% •	16%
1	D	122	42%	36%	••	18%
1	Е	122	34% 39%	%	8% •	17%
1	F	122	49%	26%	8%	16%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4843 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 1	107	Total	С	Ν	0	S	0	0	0
	A	107	821	517	145	154	5	0	0	0
1	р	108	Total	С	Ν	0	S	0	0	0
	D		832	521	147	159	5	0	0	0
1	C	102	Total	С	Ν	0	S	0	0	0
		105	797	500	142	150	5	0	0	0
1	П	100	Total	С	Ν	0	S	0	0	0
	D	100	761	479	130	147	5	0	0	0
1	F	101	Total	С	Ν	0	S	0	0	0
			737	459	126	147	5	0	0	0
1	1 F	109	Total	С	Ν	0	S	0	0	0
		102	748	465	130	148	5	0	0	U

• Molecule 1 is a protein called Cadmium efflux system accessory protein.

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	11	GLY	CYS	engineered mutation	UNP P20047
А	101	GLY	ASP	engineered mutation	UNP P20047
А	103	ALA	HIS	engineered mutation	UNP P20047
В	11	GLY	CYS	engineered mutation	UNP P20047
В	101	GLY	ASP	engineered mutation	UNP P20047
В	103	ALA	HIS	engineered mutation	UNP P20047
С	11	GLY	CYS	engineered mutation	UNP P20047
С	101	GLY	ASP	engineered mutation	UNP P20047
С	103	ALA	HIS	engineered mutation	UNP P20047
D	11	GLY	CYS	engineered mutation	UNP P20047
D	101	GLY	ASP	engineered mutation	UNP P20047
D	103	ALA	HIS	engineered mutation	UNP P20047
Е	11	GLY	CYS	engineered mutation	UNP P20047
Е	101	GLY	ASP	engineered mutation	UNP P20047
Е	103	ALA	HIS	engineered mutation	UNP P20047
F	11	GLY	CYS	engineered mutation	UNP P20047
F	101	GLY	ASP	engineered mutation	UNP P20047



Chain	Residue	Modelled	Actual	Comment	Reference
F	103	ALA	HIS	engineered mutation	UNP P20047

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Na 2 2	0	0
2	В	2	Total Na 2 2	0	0
2	F	1	Total Na 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	26	Total O 26 26	0	0
3	В	27	Total O 27 27	0	0
3	С	25	TotalO2525	0	0
3	D	24	Total O 24 24	0	0
3	Е	24	TotalO2424	0	0
3	F	16	$\begin{array}{cc} \text{Total} & \text{O} \\ 16 & 16 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Cadmium efflux system accessory protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants	89.47Å 89.47Å 148.54Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	34.30 - 2.31	Depositor
Resolution (A)	34.30 - 2.31	EDS
% Data completeness	97.3 (34.30-2.31)	Depositor
(in resolution range)	97.3 (34.30-2.31)	EDS
R _{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.39 (at 2.31 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.237 , 0.288	Depositor
n, n_{free}	0.235 , 0.287	DCC
R_{free} test set	2539 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 41.6	EDS
L-test for $twinning^2$	$< L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	0.366 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4843	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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		Bo	ond lengths	Bond angles	
WIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.46	5/828~(0.6%)	1.18	1/1114~(0.1%)
1	В	1.60	9/840~(1.1%)	1.38	6/1130~(0.5%)
1	С	1.59	7/803~(0.9%)	1.37	7/1079~(0.6%)
1	D	1.36	3/768~(0.4%)	1.18	3/1037~(0.3%)
1	Е	1.32	2/742~(0.3%)	1.17	3/1006~(0.3%)
1	F	1.22	2/754~(0.3%)	1.23	4/1021~(0.4%)
All	All	1.44	28/4735~(0.6%)	1.26	24/6387~(0.4%)

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	В	0	1
1	Е	0	2
All	All	0	3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	81	TYR	CD2-CE2	7.92	1.51	1.39
1	С	81	TYR	CD1-CE1	7.09	1.50	1.39
1	А	42	GLU	CG-CD	7.03	1.62	1.51
1	В	63	ALA	CA-CB	6.48	1.66	1.52
1	А	86	VAL	CB-CG1	-6.25	1.39	1.52
1	D	87	ASN	CB-CG	6.13	1.65	1.51
1	F	16	LYS	CD-CE	6.06	1.66	1.51
1	В	102	GLU	CD-OE1	6.03	1.32	1.25
1	В	109	MET	CB-CG	5.88	1.70	1.51
1	С	45	ALA	CA-CB	5.82	1.64	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	37	LYS	CD-CE	5.81	1.65	1.51
1	D	15	GLU	CG-CD	5.79	1.60	1.51
1	Ε	49	TYR	CD2-CE2	5.73	1.48	1.39
1	С	88	PHE	CB-CG	5.66	1.60	1.51
1	В	52	CYS	CB-SG	-5.58	1.72	1.81
1	В	37	LYS	CE-NZ	5.58	1.62	1.49
1	D	29	ILE	CB-CG2	5.55	1.70	1.52
1	В	68	VAL	CB-CG1	5.43	1.64	1.52
1	В	37	LYS	CD-CE	5.42	1.64	1.51
1	С	78	ARG	CB-CG	5.34	1.67	1.52
1	С	52	CYS	CB-SG	-5.25	1.73	1.81
1	Ε	63	ALA	CA-CB	5.19	1.63	1.52
1	F	15	GLU	CB-CG	5.17	1.61	1.52
1	А	63	ALA	CA-CB	-5.08	1.41	1.52
1	С	59	VAL	CB-CG2	-5.08	1.42	1.52
1	А	17	VAL	C-O	5.04	1.32	1.23
1	В	44	ARG	CB-CG	5.04	1.66	1.52
1	В	59	VAL	CB-CG2	5.01	1.63	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	44	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	С	28	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	F	66	LEU	CA-CB-CG	8.14	134.02	115.30
1	F	80	LEU	CA-CB-CG	8.05	133.81	115.30
1	F	16	LYS	CD-CE-NZ	6.95	127.67	111.70
1	В	35	ILE	CG1-CB-CG2	-6.86	96.30	111.40
1	В	41	ASP	CB-CG-OD1	6.65	124.28	118.30
1	С	28	ASP	CB-CG-OD1	6.64	124.28	118.30
1	С	108	MET	CG-SD-CE	-6.56	89.71	100.20
1	В	44	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	28	ASP	CB-CG-OD1	6.02	123.72	118.30
1	Е	54	ASP	CB-CG-OD1	5.90	123.61	118.30
1	Ε	19	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	F	89	ARG	N-CA-C	-5.67	95.69	111.00
1	С	110	ILE	CG1-CB-CG2	-5.61	99.06	111.40
1	С	78	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	В	101	GLY	N-CA-C	-5.55	99.23	113.10
1	Е	108	MET	CG-SD-CE	-5.30	91.72	100.20
1	С	89	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	D	89	ARG	NE-CZ-NH1	5.21	122.91	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	48	THR	CA-CB-CG2	-5.18	105.15	112.40
1	В	105	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	С	24	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	А	61	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	91	GLU	Peptide
1	Е	26	THR	Peptide
1	Е	87	ASN	Peptide

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	А	821	0	834	31	0
1	В	832	0	838	38	0
1	С	797	0	820	47	0
1	D	761	0	754	43	0
1	Е	737	0	701	54	0
1	F	748	0	707	33	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	F	1	0	0	0	0
3	А	26	0	0	6	0
3	В	27	0	0	0	0
3	С	25	0	0	1	0
3	D	24	0	0	3	0
3	Е	24	0	0	1	0
3	F	16	0	0	3	0
All	All	4843	0	4654	210	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 22.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:24:LEU:N	1:E:25:GLN:HA	1.36	1.23
1:E:23:ASP:HB3	1:E:25:GLN:CA	1.70	1.20
1:B:47:ILE:HD11	1:B:66:LEU:HD11	1.25	1.18
1:E:20:ILE:HD11	1:F:54:ASP:OD1	1.51	1.11
1:E:23:ASP:HB3	1:E:25:GLN:CB	1.80	1.10
1:E:24:LEU:N	1:E:25:GLN:CA	2.21	1.03
1:B:27:VAL:HG13	1:B:29:ILE:HD11	1.37	1.02
1:C:40:ALA:O	1:D:33:SER:HB2	1.65	0.97
1:B:27:VAL:HG13	1:B:29:ILE:CD1	1.94	0.96
1:C:88:PHE:HD1	1:C:88:PHE:O	1.47	0.95
1:F:106:GLN:O	1:F:110:ILE:HG12	1.67	0.94
1:F:49:TYR:HE1	1:F:53:GLN:OE1	1.50	0.94
1:B:27:VAL:CG1	1:B:29:ILE:HD11	1.98	0.94
1:E:23:ASP:HB3	1:E:25:GLN:HA	1.51	0.91
1:E:112:LEU:HD22	1:F:27:VAL:HG22	1.54	0.90
1:A:44:ARG:HH11	1:A:76:HIS:HD2	1.18	0.89
1:E:24:LEU:H	1:E:25:GLN:HA	0.98	0.88
1:E:23:ASP:CB	1:E:25:GLN:CB	2.54	0.86
1:B:116:LYS:O	1:B:117:GLU:HB3	1.78	0.84
1:E:23:ASP:C	1:E:26:THR:H	1.82	0.83
1:F:43:ASN:ND2	1:F:66:LEU:HD13	1.95	0.82
1:E:24:LEU:H	1:E:25:GLN:CA	1.89	0.81
1:C:88:PHE:O	1:C:88:PHE:CD1	2.33	0.81
1:E:27:VAL:HG23	1:E:29:ILE:HG12	1.62	0.78
1:A:115:LYS:HB2	3:A:146:HOH:O	1.82	0.78
1:E:17:VAL:O	1:E:21:GLN:HB3	1.84	0.77
1:E:62:ILE:O	1:E:66:LEU:HB2	1.85	0.76
1:C:81:TYR:OH	1:C:88:PHE:CE2	2.37	0.76
1:C:20:ILE:HD13	1:C:20:ILE:N	2.00	0.76
1:C:33:SER:HB3	1:D:40:ALA:O	1.84	0.76
1:A:115:LYS:HD3	1:B:35:ILE:HG13	1.69	0.74
1:C:54:ASP:OD2	1:D:16:LYS:HE3	1.87	0.74
1:A:17:VAL:O	1:A:21:GLN:HG3	1.88	0.74
1:E:23:ASP:HB3	1:E:25:GLN:C	2.08	0.74
1:E:36:LEU:HD13	1:F:39:ILE:HG13	1.70	0.74
1:C:81:TYR:HH	1:C:88:PHE:HE2	1.34	0.72
1:F:105:ARG:HH11	1:F:105:ARG:HG3	1.56	0.70
1:B:47:ILE:CD1	1:B:66:LEU:HD11	2.14	0.69
1:B:91:GLU:N	1:B:94:LEU:O	2.27	0.68
1:E:23:ASP:CB	1:E:25:GLN:HA	2.22	0.68
1:E:27:VAL:CG2	1:E:29:ILE:HG12	2.23	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:116:LYS:O	1:B:117:GLU:CB	2.41	0.67
1:F:70:ILE:HD12	3:F:130:HOH:O	1.95	0.67
1:E:42:GLU:O	1:E:46:LYS:HG3	1.95	0.66
1:F:83:GLN:HA	1:F:83:GLN:OE1	1.94	0.66
1:E:15:GLU:H	1:E:15:GLU:CD	1.98	0.66
1:E:23:ASP:C	1:E:25:GLN:HA	2.12	0.66
1:D:115:LYS:HA	3:D:132:HOH:O	1.95	0.65
1:C:33:SER:CB	1:D:40:ALA:O	2.45	0.65
1:A:115:LYS:HD3	1:B:35:ILE:CG1	2.27	0.64
1:F:33:SER:O	1:F:37:LYS:HB2	1.98	0.64
1:A:105:ARG:O	1:A:109:MET:HG2	1.96	0.63
1:B:14:GLU:O	1:B:18:ASN:HB2	1.98	0.63
1:B:17:VAL:O	1:B:21:GLN:HG3	1.97	0.63
1:F:49:TYR:CE1	1:F:53:GLN:OE1	2.42	0.63
1:D:102:GLU:O	1:D:106:GLN:HG3	1.99	0.63
1:A:44:ARG:HH11	1:A:76:HIS:CD2	2.08	0.63
1:A:44:ARG:NH1	1:A:76:HIS:HD2	1.93	0.62
1:E:18:ASN:O	1:E:22:GLY:HA3	1.99	0.62
1:C:26:THR:HG22	1:E:88:PHE:HZ	1.64	0.62
1:E:23:ASP:CB	1:E:25:GLN:CA	2.63	0.62
1:C:33:SER:O	1:C:37:LYS:HB2	1.99	0.62
1:A:112:LEU:HD22	1:B:27:VAL:CG2	2.29	0.61
1:E:55:GLU:O	1:E:98:SER:HB3	1.99	0.61
1:F:44:ARG:HB3	1:F:80:LEU:HD21	1.82	0.61
1:C:97:TYR:N	1:C:97:TYR:CD2	2.68	0.61
1:E:56:GLU:HA	1:E:97:TYR:O	2.00	0.60
1:B:116:LYS:HZ3	1:B:116:LYS:HB3	1.66	0.60
1:D:44:ARG:HB3	1:D:80:LEU:HD21	1.83	0.59
1:F:49:TYR:HD1	1:F:49:TYR:O	1.85	0.59
1:A:112:LEU:HD22	1:B:27:VAL:HG22	1.85	0.59
1:D:10:PHE:HD2	1:D:11:GLY:N	2.00	0.59
1:D:75:HIS:CD2	3:D:136:HOH:O	2.56	0.59
1:E:51:LEU:HD23	1:E:57:LEU:HD12	1.83	0.59
1:C:63:ALA:HB1	1:C:68:VAL:O	2.03	0.58
1:F:43:ASN:HD22	1:F:66:LEU:HD13	1.68	0.58
1:C:17:VAL:HG13	1:D:65:ILE:HD13	1.84	0.58
1:C:85:VAL:O	1:C:100:GLY:N	2.30	0.58
1:A:52:CYS:O	1:A:105:ARG:NH1	2.35	0.58
1:B:38:ALA:O	1:B:44:ARG:HD2	2.04	0.58
1:D:35:ILE:HG22	1:D:36:LEU:N	2.19	0.58
1:B:113:ALA:HB1	1:D:25:GLN:HG3	1.85	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	α overlap (Å)
1·C·24·LEU·CD2	1.D.49.TYB.HD2	2.16	0.57
1.E.23.ASP.C	1.E.26.THR:N	2.55	0.57
1.A.15.GLU·HB3	3·A·126·HOH·O	2.00	0.57
1.A.29.ILE.O	1.A.32.VAL.HG12	2.05	0.56
1.C.111.ALA.HB1	1.D:32:VAL:HG13	1.87	0.56
1.C.111.ALA.CB	1:D:32:VAL:HG13	2.36	0.56
1.E.32.VAL.HG13	1.E.02. VILL.IIG10	1.88	0.56
1.C.88.PHE.CD1	1.C.90.LYS.HE3	2.41	0.56
$1 \cdot C \cdot 110 \cdot ILE \cdot CG2$	1.D.103.ALA.HB1	2.36	0.56
1.B.66.LEU.HB2	1.B.68.VAL:HG22	1.88	0.56
1.E.30.SEB.O	1.E.34.GLN.HC3	2.06	0.55
$\frac{1.1.50.5111.0}{1.8.106.GLN.0}$	1.B.110.ILE.HG12	2.00	0.55
$1 \cdot B \cdot 38 \cdot \Delta L \Delta \cdot HB2$	1.B.110.ILL.IIG12	1.80	0.55
1.D.30	1.D.40.TVR.HD2	1.05	0.55
1.6.24.000.0021	1.D.45.1110.11D2	1.70	0.55
1.F. 28. Δ SP.O	1.F.31.CLV·N	2.10	0.54
1.E.20.ASI .O	1.E.51.GL1.N	2.38	0.54
1.C.56.CLU.HA	1.F.00.VAL.O	2.08	0.54
1.0.30.GLU.IIA	2·Δ·1/2·ΗΟΗ·Ο	2.07	0.54
1.F.50.VAL.CC2		2.00	0.53
1.E.39. VAL.OG2	3·E·135·HOH·O	2.01	0.53
	1. A . 18. A SN. CC	2.00	0.53
1.A.14.GLU.U	1.F.65.II F.HD12	2.47	0.53
1.E.20.1LE.11G21	1.F.05.ILE.IID15	2.08	0.52
1.0.45.A5N.0	1.0.47.ILL.IIG15	1.01	0.52
1.A.00.LEU.IIB2	3.E.120.HOH.O	2.42	0.52
1.D.44.ARG.MII	1.D.44.ABC.NH1	2.42	0.52
1.D.41.ASI .IID2	1.D.11.CIV.H	1.57	0.52
1.D.10.1 IIE.IID2	2.D.121.HOH.O	2.40	0.52
1.D.44.AIG.NII2	1.D.110.II F.HC12	2.40	0.52
1.C.30.SEB.HB2	3·C·1/3·HOH·O	2.10	0.52
1.0.30.3ER.IID2	1.F.100.CIV.HA3	2.10	0.51
1.0.04.011.0	1.D.83.CI N.OF1	2.11	0.51
1.0.11J.L1J.NZ	1.D.35.GLN.0E1	2.43	0.51
1.D.55.1LE.CG2	1.D.50.LEU.N	2.14	0.51
1.L.JI.LEU:UD2	1.1.37.112 (1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.	2.41	0.01
1.A.30.GLU.IIA	1.R.97.VAL.UC99	2.11	0.01
1.A.112.LEU:UD2 1.C.109.MET.UE?	1.D.27.VAL:IIG22	2.40	0.51
1.0.100.WE1.IE3	1.0.112.LEU.IIG	1.30 0.06	0.50
1.0.94.LEU:IID23	1.0.94.LEU.N 1.0.70.TUD.O	2.20	0.50
1.E.66.I FILIDO	1.E.69.VAL.UC22	2.40	0.30
1:F:00:LEU:HB2	1:F:08:VAL:HG22	1.95	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:73:ALA:O	1:F:77:LEU:HD12	2.13	0.49
1:C:72:ASN:O	1:C:73:ALA:C	2.50	0.49
1:E:58:CYS:O	1:E:61:ASP:HB2	2.12	0.49
1:F:105:ARG:HG3	1:F:105:ARG:NH1	2.26	0.49
1:B:35:ILE:HD12	1:B:83:GLN:HB3	1.95	0.49
1:C:19:ARG:HG2	1:C:20:ILE:HD13	1.94	0.49
1:D:61:ASP:O	1:D:65:ILE:HG12	2.13	0.49
1:A:116:LYS:NZ	3:A:146:HOH:O	2.35	0.48
1:C:88:PHE:CD1	1:C:88:PHE:C	2.87	0.48
1:B:47:ILE:N	1:B:47:ILE:HD13	2.28	0.48
1:D:60:CYS:SG	1:D:70:ILE:HD13	2.54	0.48
1:E:44:ARG:HG3	1:E:76:HIS:HD2	1.79	0.48
1:B:110:ILE:N	1:B:110:ILE:HD13	2.28	0.48
1:A:44:ARG:NH1	1:A:76:HIS:CD2	2.76	0.48
1:B:27:VAL:HG13	1:B:29:ILE:HD13	1.89	0.48
1:B:10:PHE:CD2	1:B:14:GLU:HG3	2.49	0.47
1:C:60:CYS:HB2	1:D:12:TYR:CE2	2.49	0.47
1:D:38:ALA:O	1:D:44:ARG:HD2	2.14	0.47
1:C:13:ASP:O	1:C:17:VAL:HG23	2.14	0.47
1:E:20:ILE:O	1:E:23:ASP:HB2	2.14	0.47
1:F:49:TYR:C	1:F:49:TYR:CD1	2.87	0.47
1:D:14:GLU:O	1:D:18:ASN:HB2	2.15	0.47
1:B:58:CYS:O	1:B:62:ILE:HD12	2.15	0.47
1:F:58:CYS:SG	1:F:60:CYS:HB2	2.54	0.47
1:B:78:ARG:HD3	1:B:82:LYS:HD2	1.97	0.47
1:C:88:PHE:CE1	1:C:90:LYS:HE3	2.50	0.46
1:E:30:SER:HA	1:F:42:GLU:OE1	2.15	0.46
1:E:44:ARG:HG3	1:E:76:HIS:CD2	2.51	0.46
1:C:24:LEU:HD23	1:D:49:TYR:CD2	2.51	0.46
1:D:88:PHE:C	1:D:88:PHE:CD2	2.89	0.46
1:D:56:GLU:HA	1:D:97:TYR:O	2.16	0.46
1:E:63:ALA:O	1:E:67:GLY:N	2.49	0.46
1:E:55:GLU:O	1:E:98:SER:CB	2.63	0.46
1:B:10:PHE:CE2	1:B:14:GLU:HG3	2.51	0.45
1:E:70:ILE:HG22	1:E:70:ILE:O	2.16	0.45
1:A:9:ILE:HA	3:A:136:HOH:O	2.17	0.45
1:E:17:VAL:O	1:E:21:GLN:CB	2.59	0.45
1:E:29:ILE:CG2	1:E:29:ILE:O	2.65	0.45
1:C:24:LEU:CD2	1:D:49:TYR:CD2	2.99	0.45
1:A:39:ILE:HG22	1:A:39:ILE:O	2.16	0.45
1:E:27:VAL:HG21	1:F:49:TYR:CE2	2.52	0.45



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:85:VAL:HA	1:C:104:ILE:HD13	1.99	0.44	
1:A:108:MET:HE3	1:A:112:LEU:HG	2.00	0.44	
1:B:29:ILE:HG23	1:B:29:ILE:HD12	1.67	0.44	
1:E:87:ASN:OD1	1:E:88:PHE:N	2.50	0.44	
1:B:63:ALA:HB1	1:B:68:VAL:O	2.18	0.44	
1:C:79:THR:O	1:C:82:LYS:HB3	2.17	0.44	
1:C:114:HIS:CE1	1:D:104:ILE:HD11	2.52	0.44	
1:E:59:VAL:HG23	1:E:73:ALA:O	2.18	0.44	
1:E:63:ALA:HB1	1:E:68:VAL:O	2.18	0.44	
1:C:62:ILE:H	1:C:62:ILE:HG12	1.59	0.43	
1:E:40:ALA:O	1:E:41:ASP:C	2.55	0.43	
1:B:89:ARG:O	1:B:89:ARG:HG3	2.18	0.43	
1:C:108:MET:HE1	1:D:29:ILE:HD13	2.01	0.43	
1:F:34:GLN:HG2	3:F:134:HOH:O	2.17	0.43	
1:C:81:TYR:OH	1:C:88:PHE:HE2	1.91	0.43	
1:D:35:ILE:O	1:D:38:ALA:HB3	2.19	0.43	
1:F:38:ALA:HB2	1:F:83:GLN:HG3	2.01	0.42	
1:A:35:ILE:HG13	1:A:83:GLN:HB3	2.00	0.42	
3:A:149:HOH:O	1:B:27:VAL:HG23	2.19	0.42	
1:C:115:LYS:HG2	1:D:31:GLY:HA3	2.01	0.42	
1:D:42:GLU:O	1:D:46:LYS:HG3	2.19	0.42	
1:B:58:CYS:SG	1:B:60:CYS:HB2	2.59	0.42	
1:E:105:ARG:O	1:E:109:MET:HE2	2.19	0.42	
1:D:106:GLN:O	1:D:107:ILE:C	2.57	0.42	
1:A:108:MET:O	1:A:112:LEU:HG	2.19	0.42	
1:F:35:ILE:O	1:F:35:ILE:HG13	2.19	0.42	
1:A:88:PHE:HA	1:A:96:LEU:O	2.20	0.42	
1:B:116:LYS:HB3	1:B:116:LYS:NZ	2.34	0.42	
1:C:49:TYR:CD2	1:D:24:LEU:HD23	2.54	0.42	
1:C:76:HIS:C	1:C:78:ARG:N	2.73	0.42	
1:F:46:LYS:O	1:F:47:ILE:C	2.55	0.41	
1:A:41:ASP:HB3	1:A:44:ARG:HB2	2.02	0.41	
1:B:47:ILE:HD12	1:B:62:ILE:HG23	2.03	0.41	
1:E:15:GLU:O	1:E:17:VAL:N	2.53	0.41	
1:C:112:LEU:CD2	1:D:32:VAL:CG2	2.98	0.41	
1:F:43:ASN:O	1:F:47:ILE:HD12	2.20	0.41	
1:F:49:TYR:HD1	1:F:49:TYR:C	2.23	0.41	
1:A:33:SER:HB3	1:B:40:ALA:O	2.20	0.41	
1:A:115:LYS:HE2	1:B:35:ILE:HD11	2.03	0.41	
1:F:85:VAL:HG13	1:F:104:ILE:HG21	2.03	0.41	
1:D:10:PHE:CD2	1:D:11:GLY:N	2.86	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ARG:O	1:F:109:MET:HG2	2.22	0.40
1:A:14:GLU:O	1:A:18:ASN:ND2	2.54	0.40
1:A:108:MET:CE	1:A:112:LEU:HG	2.52	0.40
1:C:64:ASN:HB3	1:D:17:VAL:HG21	2.04	0.40
1:D:33:SER:O	1:D:37:LYS:HB2	2.21	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	Perc	entiles
1	А	103/122~(84%)	96~(93%)	7~(7%)	0	100	100
1	В	106/122~(87%)	100 (94%)	6~(6%)	0	100	100
1	С	99/122~(81%)	91~(92%)	7~(7%)	1 (1%)	15	17
1	D	96/122~(79%)	88~(92%)	7~(7%)	1 (1%)	15	17
1	Ε	97/122~(80%)	83~(86%)	7~(7%)	7~(7%)	1	0
1	F	98/122~(80%)	85 (87%)	9~(9%)	4 (4%)	3	1
All	All	599/732~(82%)	543 (91%)	43 (7%)	13 (2%)	6	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	23	ASP
1	Е	24	LEU
1	Е	73	ALA
1	Е	16	LYS
1	F	65	ILE
1	F	100	GLY
1	Е	72	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	F	89	ARG
1	D	51	LEU
1	Е	74	SER
1	Е	115	LYS
1	F	82	LYS
1	С	73	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	86/103~(84%)	82~(95%)	4 (5%)	26	36
1	В	87/103~(84%)	77~(88%)	10 (12%)	5	6
1	С	85/103~(82%)	78~(92%)	7 (8%)	11	14
1	D	80/103~(78%)	72 (90%)	8 (10%)	7	8
1	Ε	73/103~(71%)	62~(85%)	11 (15%)	3	2
1	F	74/103~(72%)	64 (86%)	10 (14%)	4	3
All	All	485/618 (78%)	435 (90%)	50 (10%)	7	8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	9	ILE
1	А	32	VAL
1	А	54	ASP
1	А	116	LYS
1	В	18	ASN
1	В	33	SER
1	В	41	ASP
1	В	47	ILE
1	В	54	ASP
1	В	72	ASN
1	В	78	ARG
1	В	109	MET



Mol	Chain	Res	Type
1	В	116	LYS
1	В	117	GLU
1	С	74	SER
1	С	82	LYS
1	С	88	PHE
1	С	89	ARG
1	С	90	LYS
1	С	94	LEU
1	С	99	LEU
1	D	10	PHE
1	D	18	ASN
1	D	20	ILE
1	D	27	VAL
1	D	29	ILE
1	D	35	ILE
1	D	56	GLU
1	D	96	LEU
1	Е	13	ASP
1	Е	15	GLU
1	Е	23	ASP
1	Е	26	THR
1	Е	54	ASP
1	Е	72	ASN
1	Е	74	SER
1	Е	82	LYS
1	Е	99	LEU
1	Е	109	MET
1	Е	117	GLU
1	F	10	PHE
1	F	16	LYS
1	F	27	VAL
1	F	29	ILE
1	F	35	ILE
1	F	39	ILE
1	F	49	TYR
1	F	53	GLN
1	F	87	ASN
1	F	117	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such side chains are listed below:



Mol	Chain	Res	Type
1	А	76	HIS
1	В	72	ASN
1	С	114	HIS
1	D	43	ASN
1	Е	76	HIS
1	F	43	ASN
1	F	53	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

