Full wwPDB X-ray Structure Validation Report (i)

Jul 24, 2017 – 10:17 PM EDT

PDB ID	:	5X90
Title	:	Structure of DotL(656-783)-IcmS-IcmW-LvgA derived from Legionella pneumophila
Authors	:	Kim, H.; Kwak, M.J.; Kim, J.D.; Kim, Y.G.; Oh, B.H.
Deposited on	:	unknown
Resolution	:	2.80 Å(reported)

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

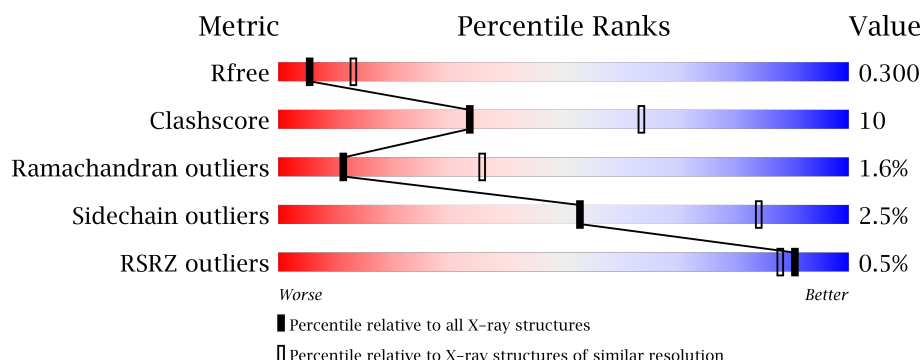|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 2.80 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	Percentile Ranks	Value
Rfree		0.300
Clashscore		10
Ramachandran outliers		1.6%
Sidechain outliers		2.5%
RSRZ outliers		0.5%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	114	83% 14% ••
1	E	114	.% 81% 18% •
2	F	149	82% 17% •
3	G	108	2% 76% 23% •
4	H	172	74% 22% ••

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Mol	Chain	Length	Quality of chain
5	B	148	73% 24%
6	C	107	2% 69% 22% 6%
7	D	171	71% 27%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8058 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 IcmS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	113	Total 849	C 540	N 135	O 165	S 9	0	0	0
1	A	113	Total 846	C 538	N 140	O 159	S 9	0	0	0

- Molecule 2 is a protein called IcmW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	149	Total 1153	C 739	N 195	O 215	S 4	0	0	0

- Molecule 3 is a protein called IcmO (DotL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	108	Total 768	C 489	N 133	O 145	S 1	0	0	0

- Molecule 4 is a protein called Hypothetical virulence protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	167	Total 1314	C 853	N 215	O 239	S 7	0	0	0

- Molecule 5 is a protein called IcmW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	146	Total 1093	C 705	N 188	O 196	S 4	0	0	0

- Molecule 6 is a protein called IcmO (DotL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	101	717	455	124	137	1	0	0	0

• Molecule 7 is a protein called Hypothetical virulence protein.

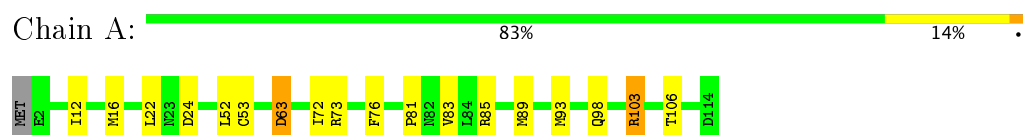| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	D	171	1318	854	221	237	6	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
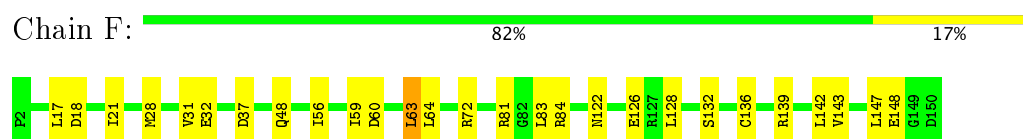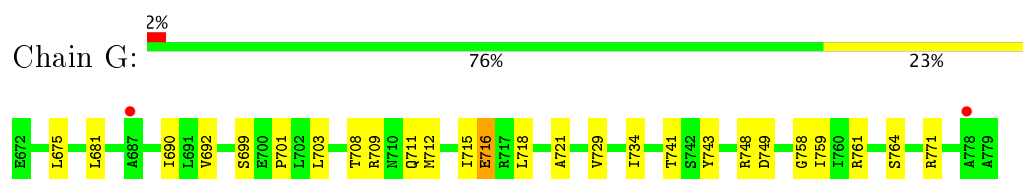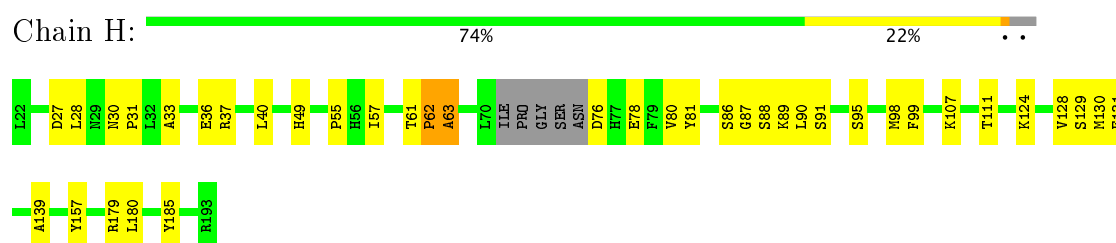
- Molecule 1: IcmS

Chain E:

- Molecule 1: IcmS

Chain A:

- Molecule 2: IcmW

Chain F:
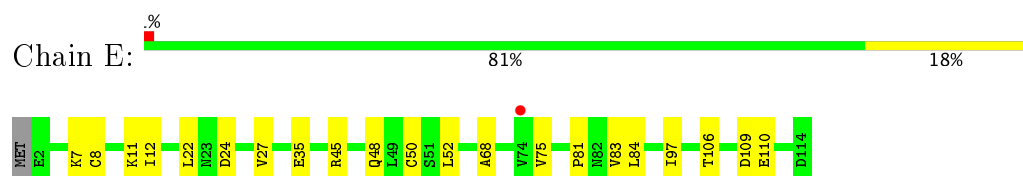
- Molecule 3: IcmO (DotL)

Chain G:

- Molecule 4: Hypothetical virulence protein

Chain H:

- Molecule 5: IcmW

Chain B:

73%　　　　24%

P2 S5 H6 E7 K11 E15 Y16 L17 I21 V24 I25 T26 F27 M28 E29 W34 E41 A45 L53 I56 I59 L64 K69 F70 I73 V74 K78 L85 D90 T91 V92 H93 P94 G95 S96 S112 ASP PRO A115 G116 F117

R127 L128 R129 C136 Q137 Y138 R139 L140 K141 L147 E148 G149

• Molecule 6: IcmO (DotL)

Chain C:

2%

69%　　　　22%　　　6%

E672 F678 L681 P688 P689 I690 L691 V692 S699 I705 I713 T714 I715 E716 R717 L718 A719 G720 K724 Y725 A726 G727 T728 V729 P744 PRO GLU GLU ARG ASP VAL I751 L756 T757 G758 I759 I760 L763 S764 A765 K766 E770 A778

• Molecule 7: Hypothetical virulence protein

Chain D:

71%　　　　27%

I25 N30 P31 L32 V35 L40 D47 F48 H49 S54 T59 I60 I64 E78 F79 V80 Y81 D85 S86 G87 S91 I92 S93 K94 S95 M98 F99 S100 K107 L108 F109 Y110 T111 I112 M115 R122 S125 G126 G127 E133 V134 F138 A139

G140 H141 Q145 R146 K147 I152 L155 N158 W169 K172 A181 Y185 S191 P192 R193 K194 I195
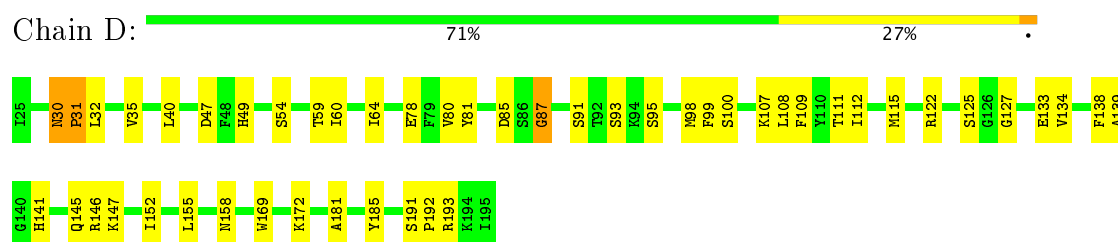
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	152.32Å 152.32Å 74.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.43 – 2.80 49.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (41.43-2.80) 95.6 (49.86-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.93 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.252 , 0.295 0.256 , 0.300	Depositor DCC
R_{free} test set	1653 reflections (3.55%)	DCC
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.1	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.034 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8058	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.36	0/859	0.61	1/1162 (0.1%)
1	E	0.38	0/862	0.57	0/1166
2	F	0.46	3/1175 (0.3%)	0.56	2/1589 (0.1%)
3	G	0.31	0/779	0.46	0/1066
4	H	0.35	0/1351	0.55	1/1836 (0.1%)
5	B	0.31	0/1113	0.54	1/1507 (0.1%)
6	C	0.34	0/726	0.57	0/989
7	D	0.35	0/1356	0.54	0/1846
All	All	0.36	3/8221 (0.0%)	0.55	5/11161 (0.0%)

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
6	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	84	ARG	CZ-NH1	-5.67	1.25	1.33
2	F	84	ARG	NE-CZ	-5.56	1.25	1.33
2	F	84	ARG	CZ-NH2	-5.37	1.26	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	64	LEU	CA-CB-CG	7.37	132.25	115.30
1	A	103	ARG	NE-CZ-NH1	-5.38	117.61	120.30
2	F	63	LEU	CA-CB-CG	5.35	127.61	115.30
2	F	64	LEU	CA-CB-CG	5.30	127.50	115.30
4	H	76	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	720	GLY	Peptide
6	C	724	LYS	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	A	846	0	829	14	0
1	E	849	0	828	13	0
2	F	1153	0	1120	24	0
3	G	768	0	746	24	0
4	H	1314	0	1257	28	0
5	B	1093	0	1049	31	0
6	C	717	0	683	24	0
7	D	1318	0	1247	36	0
All	All	8058	0	7759	154	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 10.

All (154) 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)
2:F:31:VAL:HG21	3:G:675:LEU:HD22	1.14	1.11
2:F:31:VAL:CG2	3:G:675:LEU:HD22	1.93	0.99
5:B:6:HIS:HE1	5:B:78:LYS:HD2	1.35	0.92
2:F:31:VAL:HG21	3:G:675:LEU:CD2	1.98	0.91
4:H:57:ILE:HD11	4:H:88:SER:HA	1.57	0.87
4:H:95:SER:HA	4:H:98:MET:HG3	1.54	0.86
4:H:33:ALA:HA	4:H:36:GLU:OE2	1.80	0.81
4:H:49:HIS:HB2	4:H:139:ALA:HB3	1.65	0.78
6:C:756:LEU:O	6:C:759:ILE:N	2.20	0.76
7:D:95:SER:HA	7:D:98:MET:HB2	1.67	0.75
7:D:30:ASN:H	7:D:31:PRO:HD3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:64:LEU:O	6:C:766:LYS:NZ	2.23	0.71
5:B:6:HIS:CE1	5:B:78:LYS:HD2	2.22	0.71
7:D:81:TYR:H	7:D:111:THR:CG2	2.04	0.71
5:B:29:GLU:HB2	5:B:78:LYS:HD3	1.72	0.70
1:A:83:VAL:HG22	6:C:715:ILE:HG22	1.74	0.70
7:D:81:TYR:H	7:D:111:THR:HG21	1.57	0.69
3:G:675:LEU:HD23	3:G:743:TYR:O	1.92	0.69
5:B:73:ILE:HG12	6:C:760:ILE:HG22	1.75	0.69
7:D:60:ILE:HD12	7:D:64:ILE:HD12	1.75	0.69
2:F:59:ILE:HD11	3:G:771:ARG:HB2	1.76	0.68
4:H:61:THR:HA	4:H:63:ALA:H	1.60	0.66
4:H:57:ILE:HD11	4:H:88:SER:CA	2.25	0.66
3:G:708:THR:O	3:G:712:MET:HG3	1.99	0.62
5:B:69:LYS:O	5:B:73:ILE:HD12	2.00	0.62
5:B:5:SER:OG	5:B:6:HIS:N	2.33	0.61
5:B:94:PRO:HB3	7:D:93:SER:HB3	1.82	0.61
1:E:35:GLU:CD	1:E:35:GLU:H	2.03	0.61
5:B:74:VAL:HG12	5:B:85:LEU:HD23	1.84	0.60
6:C:690:ILE:HG22	6:C:692:VAL:H	1.66	0.60
2:F:122:ASN:O	2:F:126:GLU:HG2	2.02	0.60
5:B:56:ILE:HG13	5:B:92:VAL:HG11	1.83	0.59
7:D:152:ILE:O	7:D:155:LEU:HG	2.03	0.58
1:A:81:PRO:HB3	6:C:729:VAL:HG21	1.86	0.57
5:B:59:ILE:HD11	5:B:64:LEU:HD23	1.87	0.57
5:B:129:ARG:HH21	7:D:100:SER:HA	1.69	0.57
7:D:30:ASN:H	7:D:31:PRO:CD	2.17	0.57
7:D:32:LEU:O	7:D:35:VAL:HG12	2.04	0.56
2:F:37:ASP:OD2	2:F:81:ARG:NH1	2.37	0.56
2:F:48:GLN:OE1	3:G:761:ARG:NH1	2.39	0.55
1:E:97:ILE:HA	1:E:106:THR:HG21	1.89	0.54
3:G:748:ARG:HG2	3:G:749:ASP:H	1.73	0.54
5:B:21:ILE:HD11	7:D:99:PHE:O	2.08	0.54
1:E:45:ARG:NH2	1:E:110:GLU:OE1	2.35	0.54
2:F:32:GLU:OE2	3:G:743:TYR:OH	2.22	0.54
1:E:81:PRO:HB3	3:G:729:VAL:HG11	1.90	0.54
1:E:27:VAL:HG12	4:H:185:TYR:HE2	1.72	0.54
2:F:56:ILE:HA	2:F:59:ILE:HD12	1.90	0.53
5:B:11:LYS:O	5:B:15:GLU:HG3	2.08	0.53
5:B:137:GLN:O	5:B:141:LYS:HG3	2.09	0.53
7:D:85:ASP:OD1	7:D:87:GLY:N	2.42	0.53
2:F:148:GLU:HB2	3:G:718:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:LEU:CD2	3:G:741:THR:HB	2.39	0.53
1:A:89:MET:O	1:A:93:MET:HG2	2.10	0.52
5:B:21:ILE:O	5:B:25:ILE:HG13	2.09	0.52
2:F:21:ILE:HD13	4:H:99:PHE:HB2	1.91	0.52
1:A:52:LEU:HD12	7:D:40:LEU:HD23	1.91	0.52
6:C:714:THR:O	6:C:718:LEU:HG	2.10	0.52
7:D:107:LYS:O	7:D:111:THR:HG23	2.11	0.51
7:D:138:PHE:HZ	7:D:152:ILE:HD12	1.76	0.51
6:C:681:LEU:HB3	6:C:699:SER:HB3	1.92	0.51
7:D:85:ASP:OD2	7:D:122:ARG:NH2	2.42	0.51
5:B:64:LEU:HD22	6:C:766:LYS:HZ3	1.76	0.51
1:E:83:VAL:HG21	3:G:712:MET:HB3	1.92	0.50
6:C:756:LEU:O	6:C:758:GLY:N	2.45	0.50
5:B:6:HIS:HE1	5:B:78:LYS:CD	2.18	0.49
6:C:678:PHE:CD1	6:C:705:ILE:HG12	2.47	0.49
7:D:141:HIS:O	7:D:145:GLN:HG3	2.13	0.49
1:A:83:VAL:HG22	6:C:715:ILE:CG2	2.42	0.49
5:B:129:ARG:NH2	7:D:100:SER:HA	2.28	0.49
2:F:17:LEU:HD12	2:F:18:ASP:N	2.28	0.49
4:H:80:VAL:HG23	4:H:111:THR:HA	1.95	0.49
6:C:763:LEU:O	6:C:766:LYS:N	2.46	0.48
4:H:57:ILE:HD12	4:H:57:ILE:O	2.13	0.48
5:B:45:ALA:HB1	6:C:760:ILE:HD11	1.95	0.48
5:B:147:LEU:HD11	6:C:719:ALA:HB2	1.96	0.48
1:A:24:ASP:OD1	7:D:192:PRO:HB3	2.14	0.48
3:G:709:ARG:HB2	3:G:734:ILE:CD1	2.44	0.47
1:A:98:GLN:NE2	1:A:103:ARG:HD2	2.30	0.47
4:H:95:SER:HA	4:H:98:MET:CG	2.38	0.47
3:G:711:GLN:O	3:G:715:ILE:HG13	2.15	0.47
2:F:21:ILE:CD1	4:H:99:PHE:HB2	2.44	0.47
7:D:108:LEU:O	7:D:112:ILE:HG13	2.14	0.47
7:D:54:SER:O	7:D:134:VAL:HA	2.14	0.47
7:D:138:PHE:CZ	7:D:152:ILE:HD12	2.50	0.46
7:D:146:ARG:HB3	7:D:169:TRP:CH2	2.51	0.46
2:F:132:SER:O	2:F:136:CYS:HB3	2.14	0.46
4:H:28:LEU:O	4:H:31:PRO:HD2	2.16	0.46
5:B:90:ASP:HA	5:B:96:SER:HB3	1.98	0.46
7:D:80:VAL:HB	7:D:111:THR:HG22	1.97	0.46
3:G:709:ARG:HB2	3:G:734:ILE:HD11	1.98	0.46
4:H:81:TYR:CE1	4:H:107:LYS:HD3	2.51	0.46
7:D:193:ARG:HA	7:D:193:ARG:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:CYS:SG	1:E:84:LEU:HD21	2.56	0.46
4:H:28:LEU:C	4:H:31:PRO:HD2	2.35	0.46
2:F:28:MET:O	2:F:32:GLU:HG3	2.16	0.46
4:H:61:THR:HB	4:H:62:PRO:HA	1.98	0.46
4:H:86:SER:O	4:H:88:SER:N	2.48	0.46
4:H:55:PRO:HG3	4:H:128:VAL:HG21	1.97	0.45
4:H:57:ILE:HD12	4:H:57:ILE:C	2.37	0.45
7:D:49:HIS:ND1	7:D:91:SER:HB2	2.31	0.45
1:A:12:ILE:O	1:A:16:MET:HG3	2.16	0.45
1:A:76:PHE:HB3	1:A:85:ARG:CZ	2.47	0.45
3:G:701:PRO:HB2	3:G:703:LEU:O	2.17	0.45
6:C:770:GLU:OE1	6:C:770:GLU:N	2.50	0.45
3:G:716:GLU:O	3:G:721:ALA:HB3	2.17	0.45
5:B:136:CYS:SG	5:B:139:ARG:HG2	2.57	0.44
1:E:52:LEU:HD21	2:F:126:GLU:HB2	2.00	0.44
6:C:713:ILE:HG12	6:C:726:ALA:O	2.17	0.44
2:F:72:ARG:NH2	6:C:728:THR:OG1	2.50	0.44
7:D:49:HIS:HB2	7:D:139:ALA:HB3	2.00	0.44
5:B:7:GLU:HG3	6:C:688:PRO:HB3	2.00	0.44
5:B:26:THR:O	5:B:29:GLU:HG3	2.18	0.44
1:E:81:PRO:HB3	3:G:729:VAL:CG1	2.48	0.44
4:H:124:LYS:HA	4:H:124:LYS:HD2	1.55	0.43
4:H:129:SER:O	4:H:131:GLU:N	2.51	0.43
1:E:8:CYS:O	1:E:12:ILE:HG13	2.18	0.43
5:B:115:ALA:O	5:B:117:PHE:N	2.48	0.43
6:C:716:GLU:HG3	6:C:729:VAL:HG11	2.00	0.43
4:H:89:LYS:O	4:H:90:LEU:HD23	2.18	0.43
1:A:72:ILE:HD11	7:D:172:LYS:NZ	2.33	0.43
7:D:78:GLU:HG3	7:D:80:VAL:HG22	2.00	0.43
1:E:7:LYS:O	1:E:11:LYS:HG3	2.18	0.43
7:D:122:ARG:HG3	7:D:122:ARG:HH11	1.84	0.42
2:F:128:LEU:HD23	3:G:741:THR:HB	2.00	0.42
1:A:22:LEU:HA	1:A:22:LEU:HD12	1.61	0.42
5:B:64:LEU:HD22	6:C:766:LYS:NZ	2.34	0.42
4:H:180:LEU:HD23	4:H:180:LEU:HA	1.83	0.42
1:E:52:LEU:HD13	4:H:40:LEU:HD23	2.00	0.42
7:D:30:ASN:N	7:D:31:PRO:CD	2.82	0.42
1:E:68:ALA:O	4:H:179:ARG:HD2	2.19	0.42
2:F:83:LEU:HA	2:F:83:LEU:HD23	1.86	0.42
7:D:47:ASP:HA	7:D:93:SER:HA	2.01	0.42
7:D:181:ALA:HA	7:D:185:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG23	6:C:716:GLU:HG2	2.02	0.42
6:C:681:LEU:HD21	6:C:690:ILE:HD11	2.01	0.42
7:D:109:PHE:CG	7:D:147:LYS:HG2	2.55	0.42
2:F:60:ASP:HB3	2:F:63:LEU:HD23	2.01	0.42
6:C:757:THR:HA	6:C:760:ILE:HG12	2.02	0.41
7:D:111:THR:O	7:D:115:MET:HG3	2.20	0.41
4:H:49:HIS:ND1	4:H:91:SER:HB2	2.34	0.41
2:F:143:VAL:O	2:F:147:LEU:HG	2.20	0.41
3:G:690:ILE:HG22	3:G:692:VAL:H	1.85	0.41
2:F:72:ARG:HG2	3:G:759:ILE:HD13	2.02	0.41
7:D:133:GLU:HA	7:D:158:ASN:O	2.20	0.41
5:B:53:LEU:O	5:B:56:ILE:HG12	2.21	0.41
3:G:748:ARG:HG2	3:G:749:ASP:N	2.34	0.41
4:H:157:TYR:CD1	4:H:157:TYR:N	2.88	0.41
3:G:681:LEU:HB3	3:G:699:SER:HB3	2.03	0.41
5:B:70:PHE:O	5:B:74:VAL:HG13	2.21	0.41
1:A:63:ASP:OD1	1:A:63:ASP:N	2.54	0.40
2:F:21:ILE:HD11	4:H:99:PHE:O	2.21	0.40
5:B:24:VAL:O	5:B:28:MET:HG3	2.21	0.40
1:A:53:CYS:HA	5:B:127:ARG:HG2	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	111/114 (97%)	105 (95%)	6 (5%)	0	100	100
1	E	111/114 (97%)	102 (92%)	9 (8%)	0	100	100
2	F	147/149 (99%)	134 (91%)	13 (9%)	0	100	100
3	G	106/108 (98%)	99 (93%)	6 (6%)	1 (1%)	20	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	163/172 (95%)	142 (87%)	16 (10%)	5 (3%)	5	16
5	B	142/148 (96%)	124 (87%)	15 (11%)	3 (2%)	8	27
6	C	97/107 (91%)	86 (89%)	8 (8%)	3 (3%)	5	16
7	D	169/171 (99%)	148 (88%)	16 (10%)	5 (3%)	5	17
All	All	1046/1083 (97%)	940 (90%)	89 (8%)	17 (2%)	11	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	130	MET
6	C	724	LYS
7	D	30	ASN
4	H	87	GLY
5	B	41	GLU
5	B	5	SER
5	B	34	TRP
7	D	31	PRO
4	H	63	ALA
6	C	764	SER
7	D	127	GLY
7	D	191	SER
6	C	756	LEU
3	G	758	GLY
4	H	30	ASN
7	D	87	GLY
4	H	62	PRO

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	88/97 (91%)	85 (97%)	3 (3%)	42	76
1	E	90/97 (93%)	85 (94%)	5 (6%)	25	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	118/131 (90%)	116 (98%)	2 (2%)	66	90
3	G	73/91 (80%)	71 (97%)	2 (3%)	50	83
4	H	138/152 (91%)	135 (98%)	3 (2%)	57	87
5	B	106/130 (82%)	104 (98%)	2 (2%)	62	89
6	C	66/91 (72%)	65 (98%)	1 (2%)	70	92
7	D	133/151 (88%)	131 (98%)	2 (2%)	70	92
All	All	812/940 (86%)	792 (98%)	20 (2%)	53	84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	22	LEU
1	E	24	ASP
1	E	48	GLN
1	E	75	VAL
1	E	109	ASP
2	F	139	ARG
2	F	142	LEU
3	G	716	GLU
3	G	764	SER
4	H	27	ASP
4	H	37	ARG
4	H	78	GLU
1	A	63	ASP
1	A	73	ARG
1	A	106	THR
5	B	17	LEU
5	B	129	ARG
6	C	714	THR
7	D	59	THR
7	D	125	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	98	GLN
2	F	137	GLN
4	H	145	GLN
1	A	98	GLN

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Mol	Chain	Res	Type
5	B	6	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

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, 95th 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(Å²)	Q<0.9
1	A	113/114 (99%)	-0.57	0	100	100	38, 54, 73, 81	0
1	E	113/114 (99%)	-0.51	1 (0%)	84	79	31, 54, 75, 86	0
2	F	149/149 (100%)	-0.43	0	100	100	35, 57, 86, 100	0
3	G	108/108 (100%)	-0.44	2 (1%)	67	58	46, 67, 98, 105	0
4	H	167/172 (97%)	-0.38	0	100	100	32, 58, 97, 113	0
5	B	146/148 (98%)	-0.38	0	100	100	41, 72, 96, 111	0
6	C	101/107 (94%)	-0.25	2 (1%)	65	56	46, 75, 110, 121	0
7	D	171/171 (100%)	-0.37	0	100	100	39, 63, 102, 119	0
All	All	1068/1083 (98%)	-0.41	5 (0%)	90	88	31, 61, 100, 121	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	C	759	ILE	3.2
1	E	74	VAL	2.6
3	G	687	ALA	2.3
3	G	778	ALA	2.1
6	C	763	LEU	2.0

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.