Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 06:22 AM JST

PDB ID	:	7F8M
Title	:	Roadblock from Thorarchaeota SMTZ1-45
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Deposited on	:	2021-07-02
Resolution	:	2.14 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

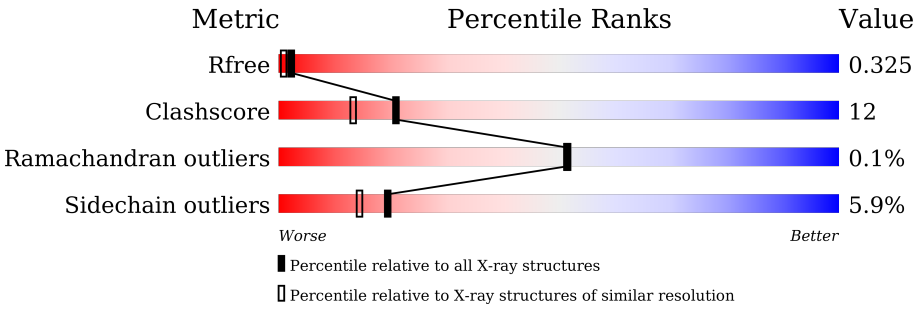
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)

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	A	120	66% 30%
1	B	120	76% 20%
1	C	120	75% 20%
1	D	120	72% 21%
1	E	120	72% 24%
1	F	120	81% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5589 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 Robl_LC7 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	2	0
			884	559	145	178	2			
1	B	120	Total	C	N	O	S	0	0	0
			888	560	147	179	2			
1	C	117	Total	C	N	O	S	0	1	0
			881	557	145	177	2			
1	D	116	Total	C	N	O	S	0	2	0
			877	556	143	176	2			
1	E	116	Total	C	N	O	S	0	3	0
			880	558	143	177	2			
1	F	116	Total	C	N	O	S	0	1	0
			873	553	143	175	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A135VIJ8
A	2	SER	-	expression tag	UNP A0A135VIJ8
A	3	SER	-	expression tag	UNP A0A135VIJ8
A	4	ALA	-	expression tag	UNP A0A135VIJ8
B	1	MET	-	initiating methionine	UNP A0A135VIJ8
B	2	SER	-	expression tag	UNP A0A135VIJ8
B	3	SER	-	expression tag	UNP A0A135VIJ8
B	4	ALA	-	expression tag	UNP A0A135VIJ8
C	1	MET	-	initiating methionine	UNP A0A135VIJ8
C	2	SER	-	expression tag	UNP A0A135VIJ8
C	3	SER	-	expression tag	UNP A0A135VIJ8
C	4	ALA	-	expression tag	UNP A0A135VIJ8
D	1	MET	-	initiating methionine	UNP A0A135VIJ8
D	2	SER	-	expression tag	UNP A0A135VIJ8
D	3	SER	-	expression tag	UNP A0A135VIJ8
D	4	ALA	-	expression tag	UNP A0A135VIJ8
E	1	MET	-	initiating methionine	UNP A0A135VIJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	SER	-	expression tag	UNP A0A135VIJ8
E	3	SER	-	expression tag	UNP A0A135VIJ8
E	4	ALA	-	expression tag	UNP A0A135VIJ8
F	1	MET	-	initiating methionine	UNP A0A135VIJ8
F	2	SER	-	expression tag	UNP A0A135VIJ8
F	3	SER	-	expression tag	UNP A0A135VIJ8
F	4	ALA	-	expression tag	UNP A0A135VIJ8

- Molecule 2 is water.

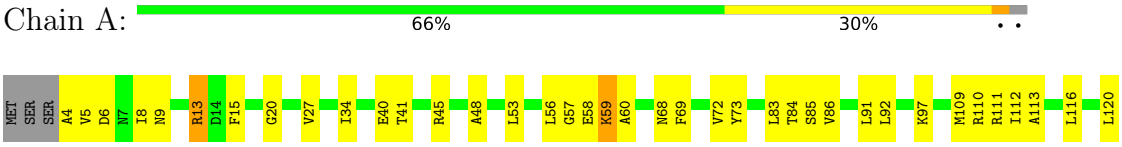
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	48	Total O 48 48	0	0
2	B	57	Total O 57 57	0	0
2	C	57	Total O 57 57	0	0
2	D	34	Total O 34 34	0	0
2	E	49	Total O 49 49	0	0
2	F	61	Total O 61 61	0	0

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.

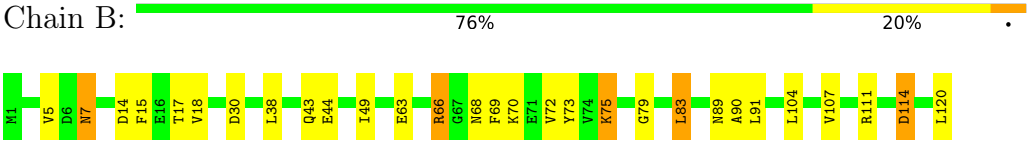
• Molecule 1: Robl_LC7 domain-containing protein

Chain A:



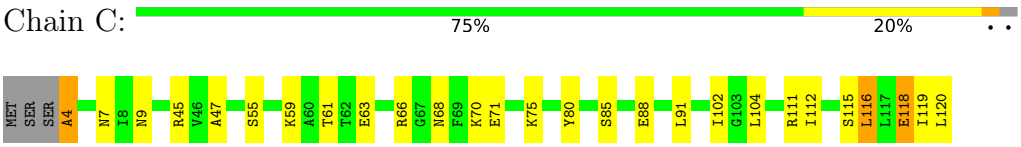
• Molecule 1: Robl_LC7 domain-containing protein

Chain B:



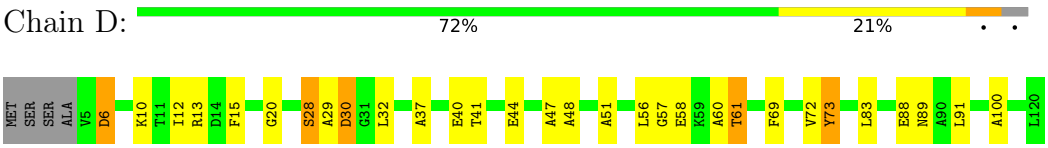
• Molecule 1: Robl_LC7 domain-containing protein

Chain C:



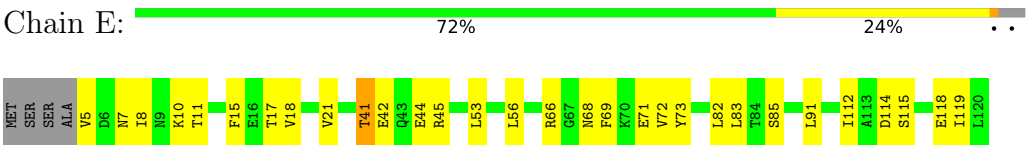
• Molecule 1: Robl_LC7 domain-containing protein

Chain D:



• Molecule 1: Robl_LC7 domain-containing protein

Chain E:



• Molecule 1: Robl_LC7 domain-containing protein

Chain F:


MET
SER
SER
ALA
V5
D6
R13
G23
L26
M33
I34
S35
S36
R45
I49
K59
Y73
L95
G103
F106
M109
S115
L116
L117
E118
I119
L120

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	58.98Å 58.98Å 193.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.14 20.04 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.14) 97.7 (20.04-2.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.191 , 0.260 0.262 , 0.325	Depositor DCC
R_{free} test set	1995 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.166 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5589	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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	0.92	0/893	1.05	0/1206
1	B	1.07	2/894 (0.2%)	1.06	1/1208 (0.1%)
1	C	1.13	4/887 (0.5%)	1.07	0/1198
1	D	0.91	0/889	1.01	1/1201 (0.1%)
1	E	0.99	0/895	1.03	1/1210 (0.1%)
1	F	1.12	4/882 (0.5%)	1.05	0/1191
All	All	1.03	10/5340 (0.2%)	1.05	3/7214 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	LEU	C-O	6.81	1.36	1.23
1	F	23	GLY	C-O	6.73	1.34	1.23
1	F	73	TYR	C-O	6.39	1.35	1.23
1	F	95	LEU	C-O	6.12	1.34	1.23
1	F	103	GLY	C-O	5.51	1.32	1.23
1	C	116	LEU	C-O	5.43	1.33	1.23
1	C	71	GLU	CD-OE1	-5.27	1.19	1.25
1	C	4	ALA	C-O	5.24	1.33	1.23
1	C	9	ASN	C-O	5.04	1.32	1.23
1	B	75	LYS	C-O	5.03	1.32	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	66	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	66	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	73	TYR	CB-CA-C	5.07	120.53	110.40

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	884	0	917	35	0
1	B	888	0	911	27	0
1	C	881	0	912	21	1
1	D	877	0	915	26	0
1	E	880	0	920	17	1
1	F	873	0	908	17	0
2	A	48	0	0	11	1
2	B	57	0	0	9	0
2	C	57	0	0	10	1
2	D	34	0	0	10	0
2	E	49	0	0	8	2
2	F	61	0	0	8	2
All	All	5589	0	5483	131	4

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 12.

All (131) 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:109:MET:SD	2:A:246:HOH:O	2.16	1.03
1:B:83:LEU:HD11	1:B:91:LEU:HD13	1.42	1.00
1:E:118:GLU:O	2:E:201:HOH:O	1.88	0.90
1:B:14:ASP:O	1:B:17:THR:HG22	1.74	0.87
1:A:111:ARG:NH1	2:A:201:HOH:O	2.14	0.81
1:C:112:ILE:O	1:C:116:LEU:HB2	1.84	0.78
1:D:44:GLU:O	2:D:201:HOH:O	2.00	0.78
1:F:116:LEU:O	2:F:201:HOH:O	2.02	0.76
1:A:45:ARG:NH2	2:A:203:HOH:O	2.18	0.76
1:D:44:GLU:OE1	2:D:202:HOH:O	2.03	0.76
1:F:13:ARG:NH1	2:F:204:HOH:O	2.20	0.74
1:D:28:SER:OG	1:D:32:LEU:O	2.06	0.73
1:A:56[A]:LEU:HD13	1:D:56:LEU:HB3	1.70	0.73
1:F:6:ASP:OD1	2:F:202:HOH:O	2.07	0.72
1:A:4:ALA:N	2:A:202:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLY:N	2:C:201:HOH:O	2.25	0.68
1:C:55:SER:OG	2:C:202:HOH:O	2.11	0.68
1:F:118:GLU:OE1	2:F:203:HOH:O	2.11	0.67
1:C:66:ARG:O	2:C:201:HOH:O	2.10	0.67
1:D:41:THR:O	2:D:203:HOH:O	2.13	0.66
1:A:97:LYS:HB2	2:A:215:HOH:O	1.94	0.66
1:E:71:GLU:OE2	2:E:202:HOH:O	2.14	0.65
1:D:29:ALA:O	2:D:204:HOH:O	2.13	0.65
1:B:44:GLU:HB2	2:B:208:HOH:O	1.97	0.64
1:C:118:GLU:OE2	2:C:203:HOH:O	2.14	0.64
1:F:116:LEU:HB2	2:F:212:HOH:O	1.97	0.64
1:B:68:ASN:HB3	2:B:245:HOH:O	1.97	0.63
1:A:56[A]:LEU:HD22	1:D:56:LEU:HD13	1.80	0.63
1:F:13:ARG:NH2	2:F:210:HOH:O	2.32	0.61
1:C:4:ALA:N	1:C:7:ASN:OD1	2.34	0.60
1:D:56:LEU:O	2:D:205:HOH:O	2.16	0.60
1:D:61:THR:HG21	1:D:69:PHE:HB2	1.83	0.60
1:B:69:PHE:HE1	1:B:72:VAL:HG23	1.67	0.58
1:D:12:ILE:HA	2:D:211:HOH:O	2.03	0.58
1:D:47:ALA:O	2:D:206:HOH:O	2.17	0.58
1:E:42:GLU:OE2	1:E:45:ARG:NH2	2.38	0.57
1:C:4:ALA:N	2:C:209:HOH:O	2.37	0.57
1:E:8:ILE:HD12	2:E:243:HOH:O	2.05	0.57
1:A:69:PHE:HZ	1:A:72:VAL:HG12	1.69	0.56
1:C:45:ARG:NH1	2:C:210:HOH:O	2.39	0.56
1:D:48:ALA:O	1:D:51:ALA:HB3	2.05	0.56
1:B:69:PHE:CE1	1:B:72:VAL:HG23	2.41	0.55
1:D:58:GLU:HA	1:D:61:THR:HG22	1.88	0.55
1:E:68:ASN:N	2:E:204:HOH:O	2.38	0.55
1:A:56[B]:LEU:HG	1:A:57:GLY:N	2.22	0.55
1:B:44:GLU:N	2:B:208:HOH:O	2.39	0.54
1:A:91:LEU:C	1:A:91:LEU:HD12	2.28	0.54
1:B:70:LYS:HD3	1:C:75:LYS:HE3	1.89	0.54
1:E:53:LEU:HD21	1:F:59:LYS:HG2	1.89	0.54
1:D:20:GLY:HA3	1:D:100:ALA:HB2	1.89	0.54
1:A:110:ARG:NH1	2:A:213:HOH:O	2.42	0.53
1:C:119:ILE:HG13	1:C:120:LEU:H	1.74	0.53
1:A:113:ALA:N	2:A:212:HOH:O	2.42	0.52
1:E:83:LEU:HD11	1:E:91:LEU:HD13	1.90	0.52
1:C:111:ARG:NH2	2:C:211:HOH:O	2.40	0.52
1:A:20:GLY:HA2	2:A:215:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ASP:OD1	1:D:6:ASP:N	2.40	0.51
1:B:90:ALA:C	2:B:205:HOH:O	2.49	0.51
1:B:114:ASP:N	1:B:114:ASP:OD1	2.44	0.50
1:A:58:GLU:OE1	2:A:204:HOH:O	2.19	0.50
1:D:72:VAL:HG12	1:D:83:LEU:HB3	1.92	0.50
1:E:5:VAL:N	2:E:213:HOH:O	2.44	0.50
1:B:15:PHE:O	1:B:18:VAL:HG13	2.11	0.50
1:E:115:SER:O	1:E:119:ILE:HG12	2.12	0.50
1:A:116:LEU:O	1:A:120:LEU:HB3	2.12	0.49
1:A:34:ILE:HD11	1:B:107:VAL:HG21	1.94	0.49
1:D:57:GLY:HA2	2:D:205:HOH:O	2.12	0.49
1:B:83:LEU:CD1	1:B:91:LEU:HD13	2.30	0.48
1:B:38:LEU:O	1:B:43:GLN:NE2	2.43	0.48
1:C:66:ARG:HB3	2:C:201:HOH:O	2.13	0.48
1:A:53:LEU:HD11	1:D:60:ALA:HB2	1.95	0.47
1:B:83:LEU:HD11	1:B:91:LEU:CD1	2.29	0.47
1:D:12:ILE:O	1:D:12:ILE:HG22	2.13	0.47
1:D:15:PHE:HB2	2:D:211:HOH:O	2.14	0.47
1:E:15:PHE:CD1	1:E:112:ILE:HD12	2.49	0.47
1:F:13:ARG:NH2	2:F:206:HOH:O	2.25	0.47
1:A:92:LEU:HD22	2:A:212:HOH:O	2.15	0.47
1:B:30:ASP:N	1:B:30:ASP:OD1	2.48	0.47
1:A:13:ARG:HD3	1:A:13:ARG:O	2.15	0.46
1:A:15:PHE:CZ	1:A:112:ILE:HD12	2.51	0.46
1:A:48:ALA:HB1	1:C:104:LEU:HD23	1.95	0.46
1:B:49:ILE:HD13	1:C:63:GLU:HB3	1.97	0.46
1:B:75:LYS:HD3	1:C:70:LYS:HE2	1.97	0.46
1:E:69:PHE:CE1	1:E:72[A]:VAL:HG23	2.51	0.46
1:A:34:ILE:CD1	1:B:107:VAL:HG21	2.46	0.46
1:D:72:VAL:CG1	1:D:83:LEU:HB3	2.46	0.46
1:C:88:GLU:O	1:C:88:GLU:HG3	2.17	0.45
1:E:21:VAL:HA	2:E:227:HOH:O	2.17	0.45
1:A:5:VAL:HA	1:A:8:ILE:HG12	1.99	0.45
1:E:41:THR:OG1	2:E:203:HOH:O	2.15	0.44
1:A:69:PHE:CZ	1:A:72:VAL:HG12	2.51	0.44
1:B:91:LEU:HA	2:B:205:HOH:O	2.16	0.44
1:B:7:ASN:HD22	1:B:7:ASN:N	2.16	0.44
1:B:89:ASN:N	2:B:204:HOH:O	2.28	0.44
1:F:13:ARG:NH2	2:F:218:HOH:O	2.51	0.44
1:C:47:ALA:HB3	2:C:224:HOH:O	2.17	0.43
1:C:80:TYR:CE1	1:C:102:ILE:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ILE:O	1:E:11:THR:HB	2.18	0.43
1:A:8:ILE:HG13	1:A:9:ASN:H	1.83	0.43
1:A:83:LEU:C	1:A:83:LEU:HD23	2.39	0.43
1:A:8:ILE:HG13	1:A:9:ASN:N	2.34	0.43
1:A:59:LYS:HG2	1:A:60:ALA:N	2.33	0.43
1:A:5:VAL:N	2:A:202:HOH:O	2.17	0.42
1:F:45:ARG:O	1:F:49:ILE:HG13	2.18	0.42
1:A:83:LEU:HD23	1:A:84:THR:N	2.35	0.42
1:F:106:PHE:HA	1:F:109:MET:HE2	1.99	0.42
1:A:86:VAL:HG12	1:A:86:VAL:O	2.19	0.42
1:C:61:THR:HA	1:C:66:ARG:HB2	2.00	0.42
1:D:10:LYS:N	2:D:207:HOH:O	2.51	0.42
1:D:91:LEU:HD12	1:D:91:LEU:C	2.40	0.42
1:B:104:LEU:HD11	2:B:222:HOH:O	2.20	0.42
1:C:59:LYS:NZ	1:C:63:GLU:OE2	2.40	0.42
1:A:5:VAL:O	1:A:9:ASN:ND2	2.53	0.42
1:F:26:LEU:O	1:F:34:ILE:HB	2.20	0.41
1:A:97:LYS:HE2	1:A:97:LYS:HB3	1.89	0.41
1:F:117:LEU:HD23	1:F:117:LEU:HA	1.85	0.41
1:D:10:LYS:HE3	1:D:10:LYS:HB2	1.88	0.41
1:A:120:LEU:O	1:B:111:ARG:HD3	2.20	0.41
1:C:68:ASN:ND2	2:C:208:HOH:O	2.34	0.41
1:B:44:GLU:CB	2:B:208:HOH:O	2.62	0.41
1:D:13:ARG:HE	1:D:37:ALA:HB2	1.86	0.41
1:C:85:SER:HA	1:C:91:LEU:HD23	2.02	0.41
1:F:33:MET:HE3	1:F:36:SER:HB3	2.03	0.41
1:F:106:PHE:CD1	1:F:109:MET:HE3	2.55	0.41
1:D:30:ASP:OD1	1:D:30:ASP:C	2.57	0.41
1:F:33:MET:CE	1:F:36:SER:HB3	2.51	0.41
1:B:30:ASP:OD2	2:B:201:HOH:O	2.22	0.40
1:E:7:ASN:ND2	2:E:214:HOH:O	2.46	0.40
1:E:56:LEU:CD1	1:F:59:LYS:HD2	2.51	0.40
1:E:82:LEU:N	1:E:82:LEU:HD12	2.37	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:214:HOH:O	2:F:255:HOH:O[1_665]	2.08	0.12
2:A:217:HOH:O	2:C:250:HOH:O[1_655]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LYS:NZ	1:E:44:GLU:OE2[2_655]	2.18	0.02
2:E:201:HOH:O	2:F:235:HOH:O[1_665]	2.19	0.01

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	117/120 (98%)	110 (94%)	7 (6%)	0	100 100
1	B	118/120 (98%)	112 (95%)	5 (4%)	1 (1%)	19 11
1	C	116/120 (97%)	113 (97%)	3 (3%)	0	100 100
1	D	116/120 (97%)	110 (95%)	6 (5%)	0	100 100
1	E	117/120 (98%)	112 (96%)	5 (4%)	0	100 100
1	F	115/120 (96%)	111 (96%)	4 (4%)	0	100 100
All	All	699/720 (97%)	668 (96%)	30 (4%)	1 (0%)	51 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	GLU

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	95/96 (99%)	87 (92%)	8 (8%)	11 6
1	B	93/96 (97%)	87 (94%)	6 (6%)	17 11
1	C	94/96 (98%)	92 (98%)	2 (2%)	53 54
1	D	95/96 (99%)	87 (92%)	8 (8%)	11 6
1	E	96/96 (100%)	88 (92%)	8 (8%)	11 6
1	F	94/96 (98%)	92 (98%)	2 (2%)	53 54
All	All	567/576 (98%)	533 (94%)	34 (6%)	19 14

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	13	ARG
1	A	40	GLU
1	A	41	THR
1	A	59	LYS
1	A	68	ASN
1	A	73	TYR
1	A	85	SER
1	B	5	VAL
1	B	7	ASN
1	B	66	ARG
1	B	73	TYR
1	B	114	ASP
1	B	120	LEU
1	C	115	SER
1	C	118	GLU
1	D	6	ASP
1	D	28	SER
1	D	30	ASP
1	D	40	GLU
1	D	61	THR
1	D	73	TYR
1	D	88	GLU
1	D	89	ASN
1	E	10	LYS
1	E	17[A]	THR
1	E	17[B]	THR

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Mol	Chain	Res	Type
1	E	18	VAL
1	E	41	THR
1	E	73	TYR
1	E	85	SER
1	E	114	ASP
1	F	106	PHE
1	F	115	SER

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

Mol	Chain	Res	Type
1	A	9	ASN
1	B	7	ASN
1	C	7	ASN
1	C	89	ASN
1	E	101	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)

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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