



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2016 – 05:11 AM EDT

PDB ID : 5CO7
Title : E. coli MazF form III
Authors : Zorzini, V.; Loris, R.
Deposited on : 2015-07-19
Resolution : 3.49 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

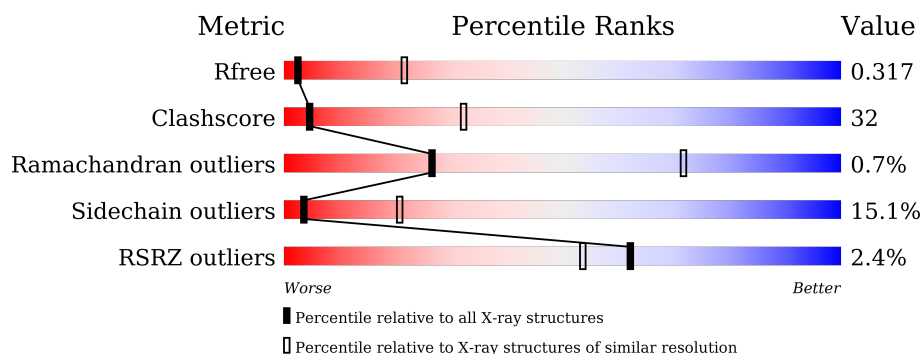
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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 $\leq 5\%$. 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	117	<div> <div>45%</div> <div>39%</div> <div>11%</div> </div>
1	B	117	<div>4%</div> <div>46%</div> <div>37%</div> <div>9%</div> <div>9%</div>
1	C	117	<div>44%</div> <div>38%</div> <div>6%</div> <div>12%</div>
1	D	117	<div>45%</div> <div>37%</div> <div>5%</div> <div>12%</div>
1	E	117	<div>5%</div> <div>56%</div> <div>31%</div> <div>7%</div> <div>6%</div>
1	F	117	<div>2%</div> <div>45%</div> <div>38%</div> <div>5%</div> <div>12%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4472 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 Endoribonuclease MazF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	1	0
			767	491	135	135	6			
1	B	107	Total	C	N	O	S	0	2	0
			765	488	133	137	7			
1	C	103	Total	C	N	O	S	0	0	0
			720	460	124	131	5			
1	D	103	Total	C	N	O	S	0	1	0
			745	479	129	130	7			
1	E	110	Total	C	N	O	S	0	0	0
			762	489	132	135	6			
1	F	103	Total	C	N	O	S	0	0	0
			713	460	125	123	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	HIS	-	expression tag	UNP P0AE70
A	113	HIS	-	expression tag	UNP P0AE70
A	114	HIS	-	expression tag	UNP P0AE70
A	115	HIS	-	expression tag	UNP P0AE70
A	116	HIS	-	expression tag	UNP P0AE70
A	117	HIS	-	expression tag	UNP P0AE70
B	112	HIS	-	expression tag	UNP P0AE70
B	113	HIS	-	expression tag	UNP P0AE70
B	114	HIS	-	expression tag	UNP P0AE70
B	115	HIS	-	expression tag	UNP P0AE70
B	116	HIS	-	expression tag	UNP P0AE70
B	117	HIS	-	expression tag	UNP P0AE70
C	112	HIS	-	expression tag	UNP P0AE70
C	113	HIS	-	expression tag	UNP P0AE70
C	114	HIS	-	expression tag	UNP P0AE70
C	115	HIS	-	expression tag	UNP P0AE70
C	116	HIS	-	expression tag	UNP P0AE70

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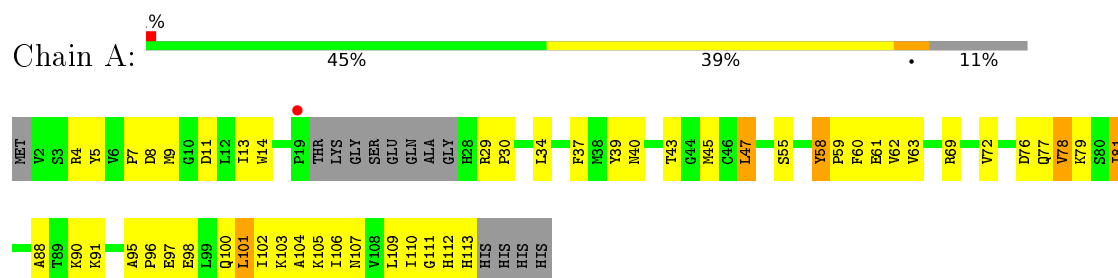
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Chain	Residue	Modelled	Actual	Comment	Reference
C	117	HIS	-	expression tag	UNP P0AE70
D	112	HIS	-	expression tag	UNP P0AE70
D	113	HIS	-	expression tag	UNP P0AE70
D	114	HIS	-	expression tag	UNP P0AE70
D	115	HIS	-	expression tag	UNP P0AE70
D	116	HIS	-	expression tag	UNP P0AE70
D	117	HIS	-	expression tag	UNP P0AE70
E	112	HIS	-	expression tag	UNP P0AE70
E	113	HIS	-	expression tag	UNP P0AE70
E	114	HIS	-	expression tag	UNP P0AE70
E	115	HIS	-	expression tag	UNP P0AE70
E	116	HIS	-	expression tag	UNP P0AE70
E	117	HIS	-	expression tag	UNP P0AE70
F	112	HIS	-	expression tag	UNP P0AE70
F	113	HIS	-	expression tag	UNP P0AE70
F	114	HIS	-	expression tag	UNP P0AE70
F	115	HIS	-	expression tag	UNP P0AE70
F	116	HIS	-	expression tag	UNP P0AE70
F	117	HIS	-	expression tag	UNP P0AE70

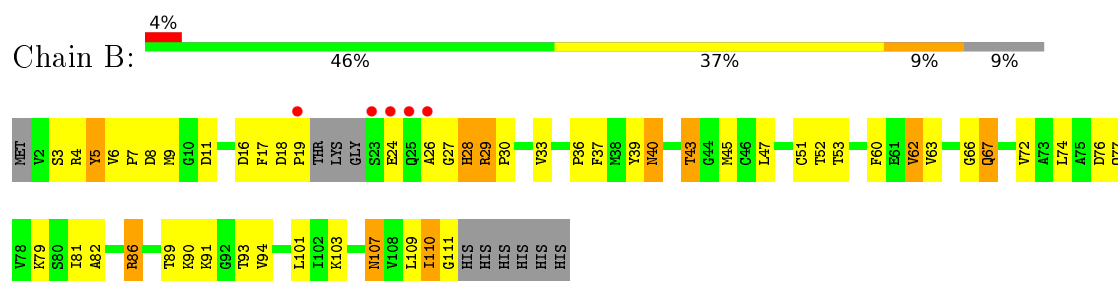
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

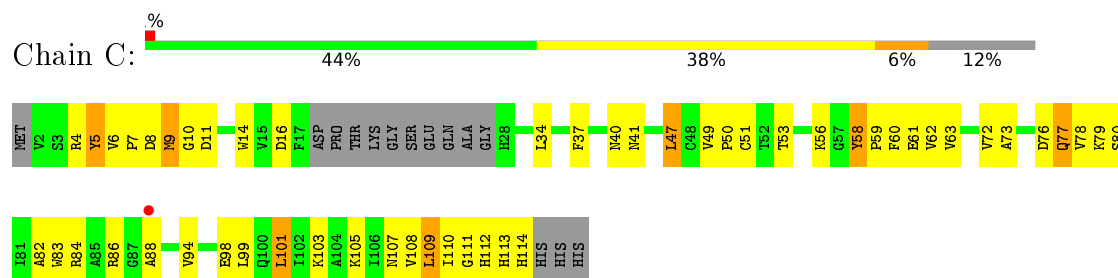
• Molecule 1: Endoribonuclease MazF



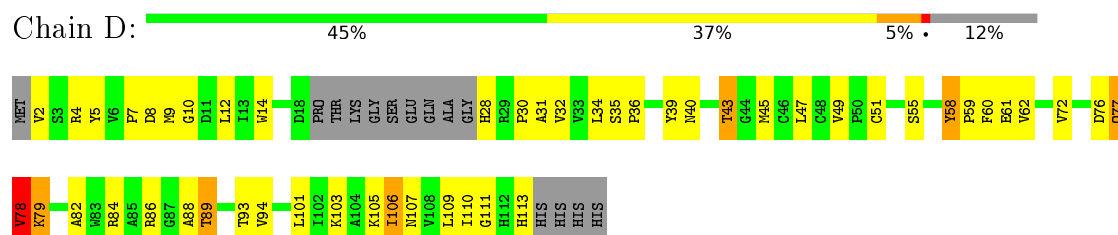
• Molecule 1: Endoribonuclease MazF



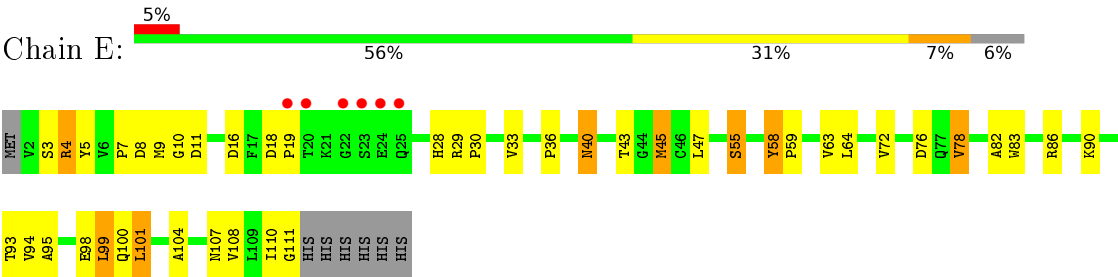
• Molecule 1: Endoribonuclease MazF



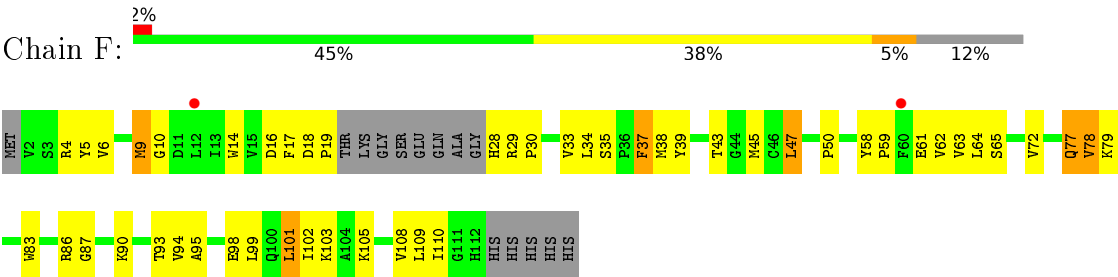
• Molecule 1: Endoribonuclease MazF



● Molecule 1: Endoribonuclease MazF



● Molecule 1: Endoribonuclease MazF



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.05Å 129.05Å 299.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.02 – 3.49 50.02 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.02-3.49) 99.4 (50.02-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.276 , 0.321 0.271 , 0.317	Depositor DCC
R_{free} test set	1641 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	128.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 141.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.46	0/784	0.71	0/1065
1	B	0.40	0/780	0.65	0/1062
1	C	0.39	0/734	0.64	0/1003
1	D	0.43	0/760	0.69	0/1034
1	E	0.42	0/778	0.67	0/1062
1	F	0.39	0/728	0.64	0/995
All	All	0.42	0/4564	0.67	0/6221

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	767	0	735	52	0
1	B	765	0	717	54	0
1	C	720	0	666	52	0
1	D	745	0	713	61	0
1	E	762	0	703	39	0
1	F	713	0	653	51	0
All	All	4472	0	4187	279	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 32.

All (279) 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:E:78:VAL:HG13	1:F:47:LEU:HD21	1.38	1.03
1:D:78:VAL:HG23	1:D:79:LYS:N	1.75	1.01
1:F:29:ARG:HG2	1:F:29:ARG:HH11	1.35	0.91
1:D:110:ILE:HG22	1:D:111:GLY:H	1.37	0.89
1:D:78:VAL:HG23	1:D:79:LYS:H	1.36	0.89
1:E:4:ARG:HG3	1:E:5:TYR:N	1.90	0.85
1:F:17:PHE:HA	1:F:86:ARG:NH2	1.91	0.84
1:F:29:ARG:HG3	1:F:30:PRO:HD2	1.60	0.82
1:F:29:ARG:CG	1:F:30:PRO:HD2	2.09	0.81
1:E:78:VAL:CG1	1:F:47:LEU:HD21	2.10	0.80
1:E:8:ASP:OD2	1:E:9:MET:N	2.16	0.79
1:F:61:GLU:HB3	1:F:72:VAL:HG21	1.66	0.77
1:D:110:ILE:HG22	1:D:111:GLY:N	1.99	0.76
1:A:4:ARG:HG3	1:A:5:TYR:N	2.00	0.76
1:A:95:ALA:HB3	1:A:98:GLU:HG3	1.67	0.76
1:B:17:PHE:HA	1:B:86:ARG:HH12	1.49	0.76
1:C:61:GLU:HB3	1:C:72:VAL:HG21	1.68	0.75
1:C:111:GLY:H	1:D:103:LYS:HD3	1.52	0.75
1:C:16:ASP:O	1:C:86:ARG:HD3	1.87	0.75
1:F:10:GLY:O	1:F:94:VAL:HG12	1.87	0.74
1:B:82:ALA:O	1:B:86:ARG:HG3	1.86	0.74
1:C:82:ALA:H	1:C:86:ARG:HH12	1.36	0.74
1:D:103:LYS:O	1:D:106:ILE:HG13	1.88	0.74
1:D:39:TYR:O	1:D:43:THR:HG23	1.88	0.73
1:A:111:GLY:O	1:A:112:HIS:ND1	2.23	0.72
1:D:60:PHE:CZ	1:D:109:LEU:HD13	2.25	0.71
1:A:107:ASN:O	1:A:111:GLY:N	2.23	0.71
1:E:99:LEU:HD12	1:E:99:LEU:O	1.91	0.71
1:F:37:PHE:C	1:F:37:PHE:HD2	1.94	0.71
1:A:4:ARG:HG3	1:A:5:TYR:H	1.54	0.70
1:C:61:GLU:HB3	1:C:72:VAL:CG2	2.20	0.70
1:B:26:ALA:HB3	1:B:29:ARG:NH2	2.07	0.69
1:D:58:TYR:OH	1:D:76:ASP:OD2	2.10	0.69
1:F:37:PHE:C	1:F:37:PHE:CD2	2.65	0.68
1:D:10:GLY:O	1:D:94:VAL:HG22	1.93	0.68
1:B:8:ASP:OD2	1:B:9:MET:N	2.27	0.67
1:A:8:ASP:O	1:A:11:ASP:HB2	1.95	0.67
1:C:82:ALA:H	1:C:86:ARG:NH1	1.91	0.67
1:F:18:ASP:N	1:F:19:PRO:HD3	2.10	0.67
1:B:62:VAL:HB	1:B:101:LEU:CD2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:VAL:CG2	1:D:79:LYS:N	2.49	0.67
1:A:39:TYR:CE1	1:A:43:THR:HG21	2.30	0.66
1:F:29:ARG:HG2	1:F:29:ARG:NH1	2.10	0.66
1:C:60:PHE:CZ	1:C:109:LEU:HD13	2.31	0.66
1:C:10:GLY:HA2	1:C:99:LEU:HD13	1.77	0.65
1:A:110:ILE:HD11	1:B:47:LEU:HD22	1.78	0.65
1:A:29:ARG:HG3	1:A:30:PRO:HD2	1.78	0.65
1:D:49:VAL:HG12	1:D:78:VAL:HA	1.79	0.65
1:F:5:TYR:CZ	1:F:90:LYS:HB2	2.32	0.65
1:C:80:SER:HB2	1:D:77:GLN:O	1.96	0.64
1:B:24:GLU:CB	1:B:77:GLN:HE22	2.11	0.64
1:B:39:TYR:CE1	1:B:43:THR:HG21	2.33	0.63
1:C:8:ASP:OD1	1:C:37:PHE:N	2.29	0.63
1:B:26:ALA:HB3	1:B:29:ARG:HH22	1.63	0.63
1:B:52:THR:HG22	1:B:74:LEU:HD11	1.81	0.63
1:C:58:TYR:HB2	1:C:59:PRO:HD2	1.81	0.63
1:D:5:TYR:O	1:D:5:TYR:CG	2.52	0.63
1:B:39:TYR:O	1:B:43:THR:HG23	1.99	0.62
1:D:61:GLU:HB3	1:D:72:VAL:HG21	1.82	0.62
1:A:58:TYR:CD1	1:A:59:PRO:HD2	2.35	0.62
1:B:36:PRO:O	1:B:40:ASN:OD1	2.17	0.62
1:C:111:GLY:N	1:D:103:LYS:HD3	2.13	0.62
1:F:4:ARG:HG3	1:F:5:TYR:N	2.15	0.62
1:E:5:TYR:CE1	1:E:7:PRO:HA	2.35	0.62
1:F:63:VAL:C	1:F:64:LEU:HD12	2.19	0.62
1:B:76:ASP:OD2	1:B:76:ASP:N	2.31	0.61
1:A:5:TYR:CZ	1:A:7:PRO:HA	2.36	0.60
1:B:17:PHE:HA	1:B:86:ARG:NH1	2.15	0.60
1:D:58:TYR:CD1	1:D:59:PRO:HD2	2.35	0.60
1:D:113:HIS:ND1	1:D:113:HIS:O	2.32	0.60
1:B:89:THR:CB	1:D:89:THR:HB	2.32	0.60
1:B:66:GLY:O	1:B:67:GLN:C	2.39	0.60
1:B:6:VAL:CB	1:B:37:PHE:HE1	2.14	0.59
1:A:81:ILE:HG12	1:A:81:ILE:O	2.01	0.59
1:A:14:TRP:CZ3	1:A:30:PRO:HD3	2.38	0.59
1:E:45:MET:HB3	1:E:82:ALA:HA	1.84	0.58
1:D:106:ILE:HD12	1:D:107:ASN:N	2.18	0.58
1:F:95:ALA:HB3	1:F:98:GLU:CB	2.34	0.57
1:C:80:SER:CB	1:D:77:GLN:O	2.52	0.57
1:E:47:LEU:HD11	1:F:109:LEU:HD23	1.85	0.57
1:B:91:LYS:HA	1:D:89:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:TYR:HB2	1:E:59:PRO:HD2	1.87	0.57
1:A:104:ALA:O	1:A:107:ASN:HB3	2.04	0.56
1:A:5:TYR:CE1	1:A:7:PRO:HA	2.40	0.56
1:B:101:LEU:C	1:B:101:LEU:HD23	2.26	0.56
1:D:106:ILE:C	1:D:106:ILE:HD12	2.25	0.56
1:D:58:TYR:HD1	1:D:59:PRO:HD2	1.70	0.56
1:B:62:VAL:HB	1:B:101:LEU:HD21	1.88	0.56
1:A:62:VAL:HG22	1:A:101:LEU:HD22	1.87	0.56
1:E:29:ARG:HG3	1:E:30:PRO:HD2	1.88	0.56
1:B:5:TYR:CZ	1:B:7:PRO:HA	2.41	0.56
1:C:58:TYR:C	1:C:58:TYR:HD1	2.08	0.56
1:B:9:MET:HA	1:B:33:VAL:HG12	1.88	0.55
1:E:76:ASP:N	1:E:76:ASP:OD2	2.39	0.55
1:C:58:TYR:C	1:C:58:TYR:CD1	2.80	0.55
1:F:29:ARG:HG2	1:F:30:PRO:HD2	1.88	0.55
1:B:40:ASN:HA	1:B:45:MET:O	2.06	0.55
1:E:4:ARG:HG3	1:E:5:TYR:H	1.71	0.55
1:B:94:VAL:HA	1:D:2:VAL:HA	1.89	0.54
1:E:4:ARG:CG	1:E:5:TYR:N	2.66	0.54
1:E:99:LEU:HD12	1:E:99:LEU:C	2.26	0.54
1:F:77:GLN:O	1:F:79:LYS:HG3	2.08	0.54
1:E:5:TYR:CZ	1:E:90:LYS:HB2	2.43	0.54
1:B:11:ASP:HA	1:B:93:THR:HG22	1.90	0.54
1:F:37:PHE:O	1:F:38:MET:C	2.45	0.54
1:C:94:VAL:HG12	1:C:98:GLU:HB2	1.90	0.54
1:D:110:ILE:CG2	1:D:111:GLY:H	2.14	0.54
1:E:9:MET:HA	1:E:33:VAL:HG12	1.89	0.54
1:E:5:TYR:CZ	1:E:7:PRO:HA	2.43	0.53
1:A:14:TRP:HZ3	1:A:30:PRO:HD3	1.71	0.53
1:A:78:VAL:CG1	1:A:106:ILE:HD13	2.38	0.53
1:E:40:ASN:N	1:E:40:ASN:OD1	2.41	0.53
1:E:95:ALA:HB3	1:E:98:GLU:HB2	1.91	0.53
1:A:58:TYR:HD1	1:A:59:PRO:HD2	1.73	0.53
1:A:61:GLU:HG2	1:A:72:VAL:HG21	1.91	0.53
1:D:35:SER:HB2	1:D:47:LEU:H	1.73	0.52
1:D:78:VAL:O	1:D:79:LYS:HG2	2.08	0.52
1:D:12:LEU:HD12	1:D:31:ALA:O	2.09	0.52
1:A:110:ILE:HD11	1:B:47:LEU:CD2	2.39	0.52
1:A:76:ASP:O	1:B:47:LEU:HD11	2.10	0.52
1:D:14:TRP:CZ3	1:D:30:PRO:HD3	2.45	0.52
1:C:50:PRO:CD	1:C:77:GLN:HB3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:VAL:HA	1:E:72:VAL:HG12	1.92	0.51
1:B:107:ASN:O	1:B:110:ILE:O	2.28	0.51
1:C:8:ASP:N	1:C:11:ASP:OD2	2.38	0.51
1:A:107:ASN:OD1	1:A:111:GLY:HA2	2.11	0.51
1:C:60:PHE:HZ	1:C:109:LEU:HD13	1.74	0.51
1:B:52:THR:HG23	1:B:72:VAL:HG13	1.92	0.51
1:C:58:TYR:CB	1:C:59:PRO:HD2	2.41	0.51
1:C:103:LYS:HD3	1:D:111:GLY:H	1.75	0.51
1:E:16:ASP:HA	1:E:28:HIS:HA	1.93	0.51
1:C:6:VAL:HG21	1:C:41:ASN:ND2	2.26	0.51
1:E:36:PRO:O	1:E:40:ASN:OD1	2.29	0.50
1:A:40:ASN:HA	1:A:45:MET:O	2.10	0.50
1:D:82:ALA:H	1:D:86:ARG:HH12	1.58	0.50
1:A:37:PHE:CD1	1:A:37:PHE:C	2.85	0.50
1:C:47:LEU:HD21	1:D:76:ASP:O	2.11	0.50
1:F:29:ARG:CG	1:F:29:ARG:HH11	2.15	0.50
1:F:35:SER:HB3	1:F:47:LEU:HB2	1.93	0.50
1:E:45:MET:HA	1:E:83:TRP:CD1	2.47	0.50
1:A:14:TRP:CE3	1:A:91:LYS:HE3	2.47	0.49
1:C:10:GLY:O	1:C:94:VAL:HG23	2.12	0.49
1:F:4:ARG:NH1	1:F:87:GLY:HA2	2.27	0.49
1:A:103[B]:LYS:HD3	1:B:111:GLY:H	1.76	0.49
1:A:78:VAL:HG11	1:A:106:ILE:HD13	1.94	0.49
1:A:58:TYR:OH	1:A:76:ASP:CG	2.51	0.49
1:B:16:ASP:O	1:B:17:PHE:C	2.49	0.49
1:D:77:GLN:O	1:D:78:VAL:HG22	2.13	0.49
1:C:49:VAL:HG12	1:C:78:VAL:HA	1.95	0.49
1:B:16:ASP:HA	1:B:28:HIS:CD2	2.48	0.49
1:D:31:ALA:HB1	1:D:49:VAL:O	2.11	0.49
1:C:50:PRO:HD2	1:C:77:GLN:HB3	1.95	0.49
1:E:64:LEU:CD2	1:E:98:GLU:HG2	2.43	0.49
1:C:49:VAL:CG1	1:C:78:VAL:HG12	2.43	0.49
1:C:114:HIS:O	1:C:114:HIS:ND1	2.46	0.49
1:F:58:TYR:HD1	1:F:59:PRO:HD2	1.78	0.49
1:A:5:TYR:CE2	1:A:90:LYS:HB2	2.48	0.48
1:C:5:TYR:CD1	1:C:5:TYR:C	2.85	0.48
1:B:17:PHE:CA	1:B:86:ARG:HH12	2.24	0.48
1:F:105:LYS:O	1:F:108:VAL:HB	2.13	0.48
1:A:60:PHE:CZ	1:A:109:LEU:HD13	2.49	0.48
1:C:107:ASN:ND2	1:D:113:HIS:HA	2.28	0.48
1:D:62:VAL:HG13	1:D:101:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:VAL:HG23	1:D:51:CYS:SG	2.54	0.48
1:E:101:LEU:O	1:E:104:ALA:HB3	2.14	0.48
1:F:9:MET:HE2	1:F:34:LEU:O	2.14	0.48
1:D:93:THR:CG2	1:D:94:VAL:N	2.76	0.48
1:C:101:LEU:HD21	1:C:105:LYS:HE3	1.95	0.48
1:D:59:PRO:O	1:D:105:LYS:HE2	2.14	0.48
1:E:19:PRO:HB3	1:E:86:ARG:HH21	1.79	0.48
1:B:39:TYR:CZ	1:B:43:THR:HG21	2.49	0.47
1:B:16:ASP:CB	1:B:86:ARG:HB3	2.43	0.47
1:E:58:TYR:CB	1:E:59:PRO:HD2	2.43	0.47
1:C:4:ARG:HG3	1:C:5:TYR:N	2.30	0.47
1:C:50:PRO:CG	1:C:77:GLN:HB3	2.44	0.47
1:D:36:PRO:O	1:D:40:ASN:ND2	2.47	0.47
1:F:50:PRO:HD2	1:F:77:GLN:HB3	1.96	0.47
1:C:49:VAL:HG12	1:C:78:VAL:HG12	1.95	0.47
1:D:55:SER:HA	1:D:72:VAL:HG11	1.96	0.47
1:F:64:LEU:HD12	1:F:64:LEU:N	2.30	0.47
1:D:82:ALA:H	1:D:86:ARG:NH1	2.12	0.47
1:D:88:ALA:O	1:D:89:THR:HG23	2.14	0.46
1:A:55:SER:OG	1:A:55:SER:O	2.32	0.46
1:D:78:VAL:O	1:D:79:LYS:CG	2.63	0.46
1:A:61:GLU:HB3	1:A:72:VAL:HG21	1.96	0.46
1:D:5:TYR:CE1	1:D:7:PRO:HA	2.50	0.46
1:F:17:PHE:HA	1:F:86:ARG:HH22	1.78	0.46
1:F:4:ARG:CG	1:F:5:TYR:N	2.79	0.46
1:A:102:ILE:O	1:A:106:ILE:HG13	2.16	0.46
1:B:60:PHE:CZ	1:B:109:LEU:HG	2.51	0.46
1:E:110:ILE:HG22	1:E:111:GLY:N	2.31	0.46
1:A:47:LEU:HD21	1:B:76:ASP:O	2.16	0.45
1:E:47:LEU:HD21	1:F:78:VAL:HG13	1.98	0.45
1:A:103[B]:LYS:HD3	1:B:110:ILE:HG22	1.97	0.45
1:B:18:ASP:N	1:B:19:PRO:HD3	2.30	0.45
1:B:5:TYR:CE2	1:B:90:LYS:HB2	2.51	0.45
1:B:9:MET:HB2	1:B:9:MET:HE2	1.82	0.45
1:E:5:TYR:CE2	1:E:90:LYS:HB2	2.52	0.45
1:F:16:ASP:HA	1:F:28:HIS:HA	1.99	0.45
1:A:39:TYR:CG	1:B:109:LEU:HD21	2.51	0.45
1:A:39:TYR:OH	1:B:76:ASP:HB2	2.18	0.44
1:B:66:GLY:O	1:B:67:GLN:O	2.35	0.44
1:C:6:VAL:HG22	1:C:83:TRP:CH2	2.52	0.44
1:C:40:ASN:N	1:C:40:ASN:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ASP:N	1:E:19:PRO:CD	2.80	0.44
1:E:43:THR:O	1:E:45:MET:HG2	2.18	0.44
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.71	0.44
1:D:35:SER:CB	1:D:47:LEU:H	2.31	0.44
1:A:110:ILE:O	1:B:103:LYS:HE2	2.17	0.44
1:F:58:TYR:CD1	1:F:59:PRO:HD2	2.53	0.44
1:A:47:LEU:HD23	1:A:47:LEU:N	2.32	0.44
1:B:3[A]:SER:N	1:D:93:THR:O	2.51	0.44
1:C:34:LEU:HA	1:C:34:LEU:HD23	1.91	0.43
1:D:76:ASP:N	1:D:76:ASP:OD1	2.49	0.43
1:F:14:TRP:CZ3	1:F:30:PRO:HD3	2.52	0.43
1:F:18:ASP:N	1:F:19:PRO:CD	2.79	0.43
1:F:62:VAL:HG21	1:F:102:ILE:HA	2.00	0.43
1:E:47:LEU:HD13	1:F:110:ILE:HD11	2.00	0.43
1:C:14:TRP:O	1:C:88:ALA:HA	2.19	0.43
1:F:17:PHE:HA	1:F:86:ARG:HH21	1.79	0.43
1:D:34:LEU:HD23	1:D:34:LEU:HA	1.86	0.43
1:A:13:ILE:HD12	1:A:88:ALA:HB1	1.99	0.43
1:B:27:GLY:HA2	1:B:28:HIS:C	2.38	0.43
1:B:39:TYR:CD1	1:B:43:THR:HG21	2.53	0.43
1:F:99:LEU:O	1:F:99:LEU:HD12	2.19	0.43
1:C:56:LYS:N	1:C:61:GLU:OE2	2.52	0.43
1:E:47:LEU:CD1	1:F:109:LEU:HD23	2.48	0.43
1:A:100:GLN:O	1:A:103[A]:LYS:HB2	2.19	0.42
1:F:50:PRO:CD	1:F:77:GLN:HB3	2.48	0.42
1:D:61:GLU:HB3	1:D:72:VAL:CG2	2.48	0.42
1:F:101:LEU:HD22	1:F:101:LEU:HA	1.60	0.42
1:D:39:TYR:CZ	1:D:43:THR:HG21	2.54	0.42
1:D:8:ASP:O	1:D:9:MET:C	2.57	0.42
1:A:4:ARG:CG	1:A:5:TYR:N	2.78	0.42
1:F:9:MET:HA	1:F:33:VAL:HG12	2.02	0.42
1:B:89:THR:CB	1:D:89:THR:CB	2.97	0.42
1:D:58:TYR:OH	1:D:76:ASP:CG	2.58	0.42
1:A:112:HIS:O	1:A:113:HIS:HB2	2.20	0.42
1:B:79:LYS:HE2	1:B:79:LYS:HB3	1.68	0.42
1:C:108:VAL:HG12	1:C:109:LEU:N	2.34	0.42
1:E:58:TYR:HD1	1:E:59:PRO:CD	2.33	0.42
1:F:39:TYR:CE1	1:F:43:THR:HG21	2.55	0.42
1:A:34:LEU:HD22	1:A:103[B]:LYS:HE2	2.02	0.42
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.67	0.42
1:C:79:LYS:HB3	1:C:79:LYS:HE3	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ILE:O	1:D:107:ASN:C	2.56	0.42
1:A:63:VAL:HG13	1:A:63:VAL:O	2.20	0.42
1:D:4:ARG:O	1:D:5:TYR:HB3	2.20	0.42
1:E:110:ILE:HG23	1:F:103:LYS:HG2	2.02	0.42
1:E:8:ASP:O	1:E:11:ASP:HB2	2.19	0.41
1:C:83:TRP:CZ2	1:C:84:ARG:HG3	2.54	0.41
1:F:63:VAL:HG22	1:F:64:LEU:N	2.36	0.41
1:C:9:MET:HE2	1:C:9:MET:HB2	1.72	0.41
1:F:6:VAL:HA	1:F:83:TRP:CH2	2.55	0.41
1:A:101:LEU:CD2	1:A:105:LYS:HE3	2.50	0.41
1:C:76:ASP:O	1:D:47:LEU:HD21	2.20	0.41
1:B:30:PRO:HG2	1:B:51:CYS:HB2	2.02	0.41
1:E:10:GLY:O	1:E:94:VAL:HG22	2.19	0.41
1:F:58:TYR:HB2	1:F:59:PRO:HD2	2.02	0.41
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.85	0.41
1:C:103:LYS:HD3	1:D:110:ILE:HG22	2.03	0.41
1:A:61:GLU:CB	1:A:72:VAL:HG21	2.51	0.41
1:A:96:PRO:HD2	1:A:97:GLU:OE1	2.21	0.41
1:B:27:GLY:HA2	1:B:29:ARG:N	2.36	0.41
1:B:16:ASP:HA	1:B:28:HIS:NE2	2.34	0.41
1:D:35:SER:HB3	1:D:40:ASN:OD1	2.21	0.41
1:F:94:VAL:HG22	1:F:95:ALA:N	2.36	0.41
1:C:5:TYR:CZ	1:C:7:PRO:HA	2.55	0.41
1:A:58:TYR:OH	1:A:76:ASP:OD2	2.37	0.40
1:B:17:PHE:HE2	1:B:79:LYS:HD3	1.86	0.40
1:C:4:ARG:HD2	1:C:5:TYR:H	1.86	0.40
1:E:55:SER:O	1:E:55:SER:OG	2.38	0.40
1:C:62:VAL:HG13	1:C:101:LEU:HD13	2.03	0.40
1:C:111:GLY:O	1:C:112:HIS:CB	2.67	0.40
1:C:113:HIS:O	1:C:114:HIS:C	2.59	0.40
1:C:51:CYS:HA	1:C:73:ALA:HA	2.01	0.40
1:D:40:ASN:HA	1:D:45:MET:O	2.22	0.40
1:F:4:ARG:HG3	1:F:5:TYR:H	1.87	0.40
1:F:4:ARG:HD2	1:F:5:TYR:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	101/117 (86%)	96 (95%)	5 (5%)	0	100	100
1	B	105/117 (90%)	97 (92%)	7 (7%)	1 (1%)	19	65
1	C	99/117 (85%)	92 (93%)	6 (6%)	1 (1%)	19	65
1	D	100/117 (86%)	86 (86%)	12 (12%)	2 (2%)	9	50
1	E	108/117 (92%)	92 (85%)	16 (15%)	0	100	100
1	F	99/117 (85%)	90 (91%)	9 (9%)	0	100	100
All	All	612/702 (87%)	553 (90%)	55 (9%)	4 (1%)	26	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	GLN
1	D	78	VAL
1	D	79	LYS
1	C	110	ILE

5.3.2 Protein sidechains

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	74/98 (76%)	65 (88%)	9 (12%)	6	29
1	B	71/98 (72%)	58 (82%)	13 (18%)	2	11
1	C	66/98 (67%)	57 (86%)	9 (14%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	70/98 (71%)	62 (89%)	8 (11%)	7	33
1	E	66/98 (67%)	53 (80%)	13 (20%)	1	9
1	F	61/98 (62%)	52 (85%)	9 (15%)	4	21
All	All	408/588 (69%)	347 (85%)	61 (15%)	3	21

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	47	LEU
1	A	58	TYR
1	A	69	ARG
1	A	77	GLN
1	A	78	VAL
1	A	79	LYS
1	A	81	ILE
1	A	101	LEU
1	B	4	ARG
1	B	5	TYR
1	B	28	HIS
1	B	29	ARG
1	B	40	ASN
1	B	43	THR
1	B	53	THR
1	B	62	VAL
1	B	63	VAL
1	B	81	ILE
1	B	86	ARG
1	B	107	ASN
1	B	110	ILE
1	C	5	TYR
1	C	9	MET
1	C	47	LEU
1	C	53	THR
1	C	58	TYR
1	C	63	VAL
1	C	77	GLN
1	C	101	LEU
1	C	109	LEU
1	D	28	HIS
1	D	43	THR

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Mol	Chain	Res	Type
1	D	58	TYR
1	D	77	GLN
1	D	78	VAL
1	D	84	ARG
1	D	89	THR
1	D	106	ILE
1	E	3	SER
1	E	4	ARG
1	E	40	ASN
1	E	45	MET
1	E	55	SER
1	E	58	TYR
1	E	78	VAL
1	E	93	THR
1	E	99	LEU
1	E	100	GLN
1	E	101	LEU
1	E	107	ASN
1	E	108	VAL
1	F	9	MET
1	F	37	PHE
1	F	45	MET
1	F	47	LEU
1	F	65	SER
1	F	77	GLN
1	F	78	VAL
1	F	93	THR
1	F	101	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	77	GLN

5.3.3 RNA ⓘ

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

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, 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(Å ²)	Q<0.9
1	A	104/117 (88%)	0.02	1 (0%) 84 77	82, 109, 176, 211	0
1	B	107/117 (91%)	0.38	5 (4%) 35 29	86, 111, 204, 252	0
1	C	103/117 (88%)	0.17	1 (0%) 84 77	94, 124, 184, 221	0
1	D	103/117 (88%)	0.07	0 100 100	94, 124, 180, 213	0
1	E	110/117 (94%)	0.24	6 (5%) 29 24	87, 112, 263, 301	0
1	F	103/117 (88%)	0.23	2 (1%) 70 62	96, 121, 178, 223	0
All	All	630/702 (89%)	0.19	15 (2%) 62 53	82, 118, 189, 301	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	GLN	6.9
1	B	26	ALA	5.2
1	E	20	THR	4.9
1	E	22	GLY	4.8
1	E	19	PRO	3.8
1	E	25	GLN	3.5
1	E	24	GLU	3.5
1	E	23	SER	3.2
1	B	24	GLU	2.3
1	A	19	PRO	2.2
1	B	23	SER	2.2
1	F	12	LEU	2.1
1	C	88	ALA	2.1
1	F	60	PHE	2.0
1	B	19	PRO	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.