Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 03:44 am BST

PDB ID	:	6FSP
Title	:	Crystal structure of APRT from Thermus thermophilus
Authors	:	Timofeev, V.I.; Sinitsyna, E.V.; Kostromina, M.A.; Muravieva, T.I.; Makarov, D.A.; Mikheeva, O.O.; Kuranova, I.P.; Esipov, R.S.
Deposited on	:	2018-02-20
Resolution	:	2.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

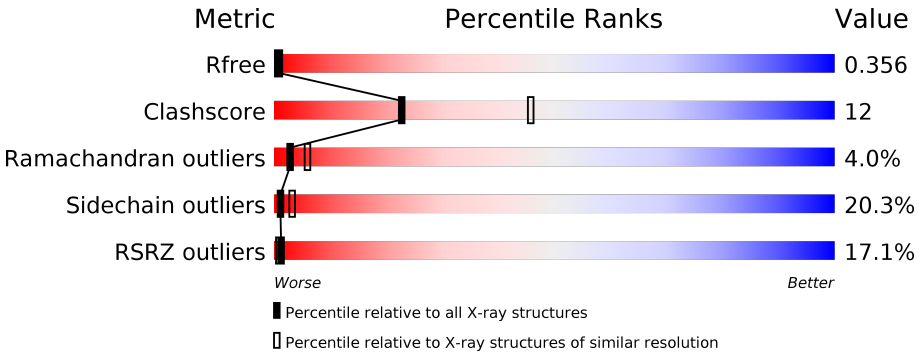
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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% 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	174	10% 61% 27% 10%
1	B	174	13% 55% 34% 7%
1	C	174	29% 67% 25% 6%
1	D	174	13% 59% 31% 10%
1	E	174	21% 68% 27% 5%
1	F	174	16% 63% 29% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7731 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.

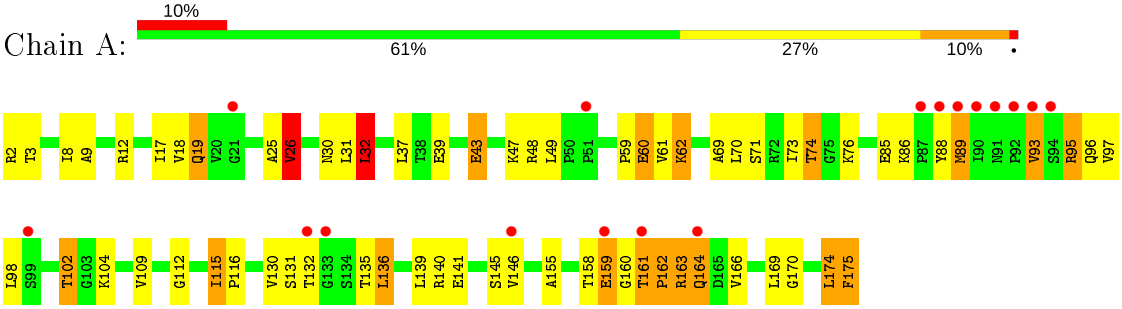
- Molecule 1 is a protein called PRPP-binding protein, adenine/guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1297	831	225	240	1			
1	B	174	Total	C	N	O	S	0	0	0
			1297	831	225	240	1			
1	C	171	Total	C	N	O	S	0	0	0
			1266	810	219	236	1			
1	D	174	Total	C	N	O	S	0	0	0
			1297	831	225	240	1			
1	E	174	Total	C	N	O	S	0	0	0
			1297	831	225	240	1			
1	F	172	Total	C	N	O	S	0	0	0
			1277	816	223	237	1			

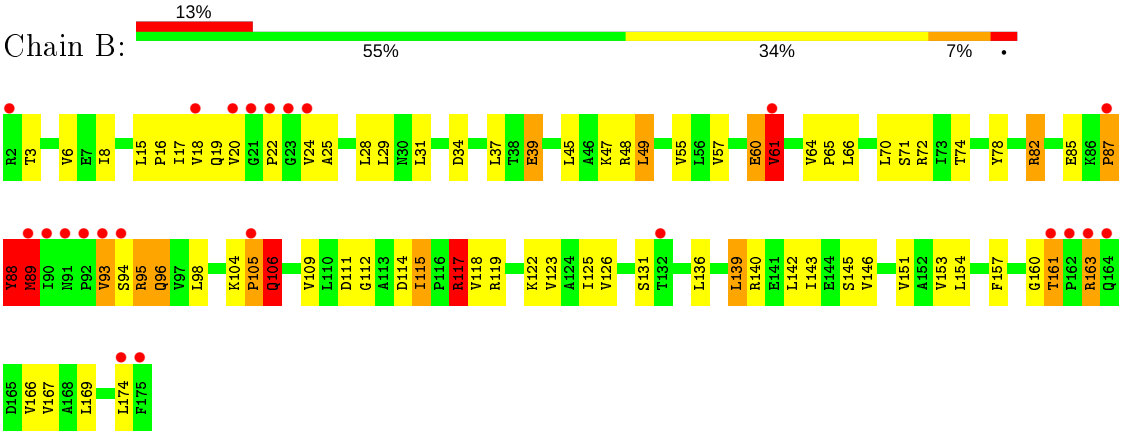
3 Residue-property plots (i)

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

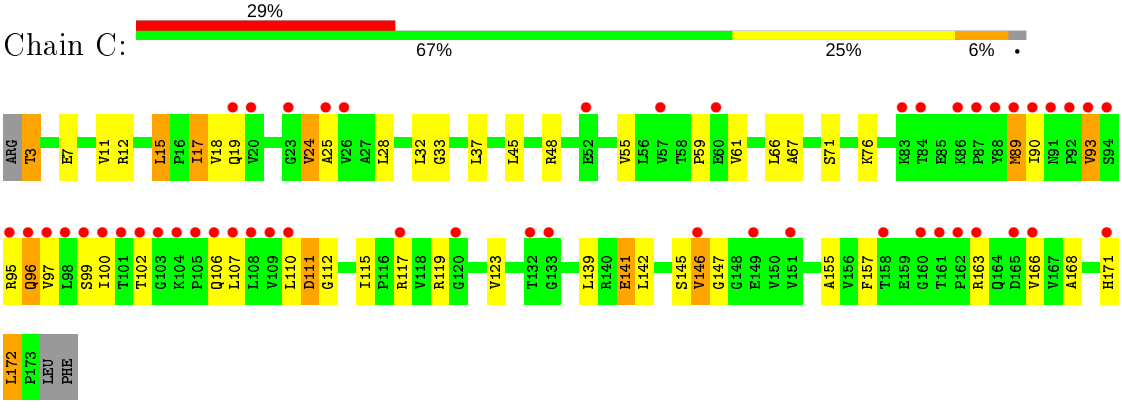
• Molecule 1: PRPP-binding protein, adenine/guanine phosphoribosyltransferase



• Molecule 1: PRPP-binding protein, adenine/guanine phosphoribosyltransferase

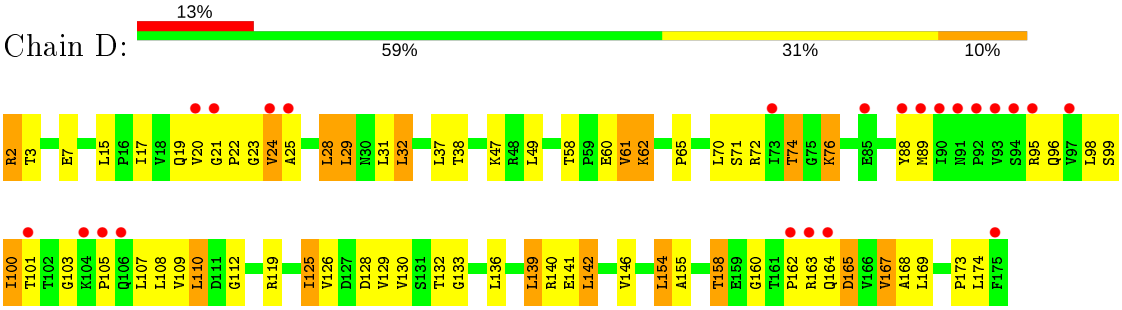


• Molecule 1: PRPP-binding protein, adenine/guanine phosphoribosyltransferase



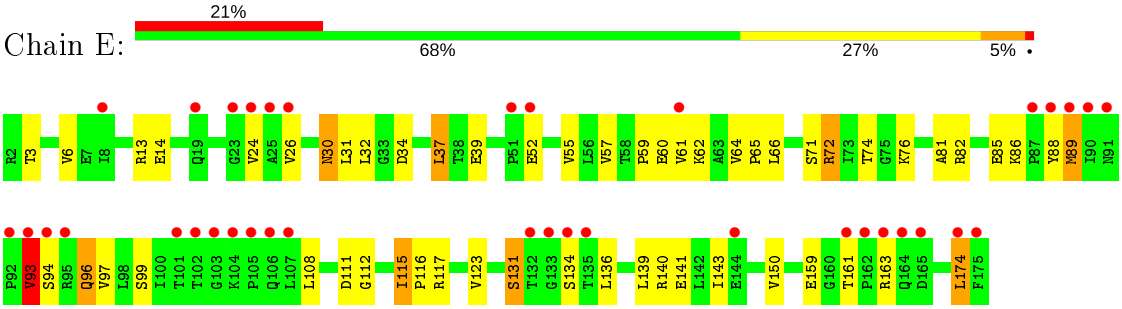
• Molecule 1: PRPP-binding protein, adenine/guanine phosphoribosyltransferase

Chain D:



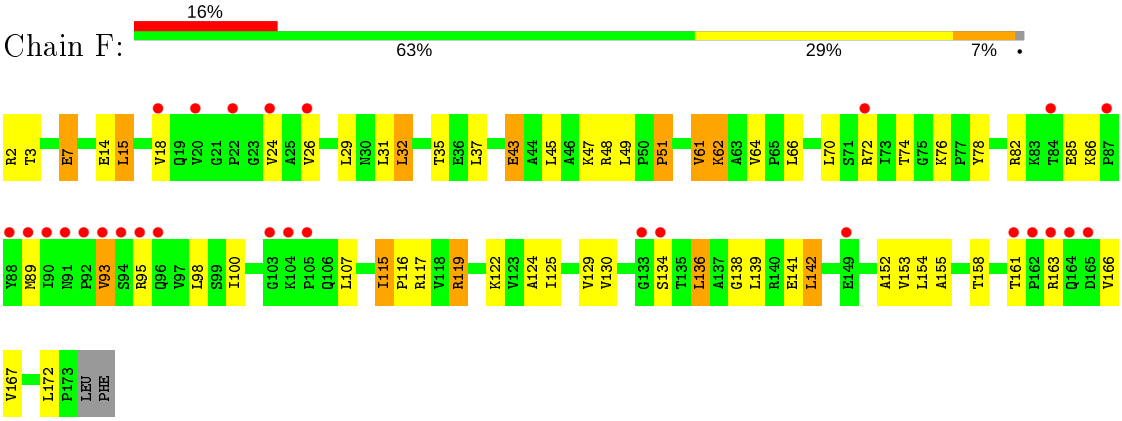
• Molecule 1: PRPP-binding protein, adenine/guanine phosphoribosyltransferase

Chain E:



• Molecule 1: PRPP-binding protein, adenine/guanine phosphoribosyltransferase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.86Å 82.16Å 91.39Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.00-2.70) 96.5 (19.95-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.10 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.248 , 0.271 0.290 , 0.356	Depositor DCC
R_{free} test set	1354 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	7731	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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	0.78	0/1317	1.03	1/1799 (0.1%)
1	B	0.83	0/1317	1.06	6/1799 (0.3%)
1	C	0.70	0/1285	0.92	0/1758
1	D	0.91	0/1317	1.07	2/1799 (0.1%)
1	E	0.75	0/1317	0.96	1/1799 (0.1%)
1	F	0.83	1/1296 (0.1%)	1.04	1/1772 (0.1%)
All	All	0.81	1/7849 (0.0%)	1.01	11/10726 (0.1%)

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	A	0	1
1	B	0	6
1	C	0	2
1	D	0	6
1	E	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	7	GLU	CD-OE2	6.65	1.32	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ASP	CB-CG-OD1	8.45	125.90	118.30
1	A	140	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	117	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	E	72	ARG	NE-CZ-NH1	6.20	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	82	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	2	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	60	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	B	119	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	82	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	72	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	82	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	VAL	Peptide
1	B	104	LYS	Peptide
1	B	106	GLN	Peptide
1	B	61	VAL	Peptide
1	B	87	PRO	Peptide
1	B	88	TYR	Peptide
1	B	93	VAL	Peptide
1	C	19	GLN	Peptide
1	C	33	GLY	Peptide
1	D	130	VAL	Peptide
1	D	160	GLY	Peptide
1	D	165	ASP	Peptide
1	D	173	PRO	Peptide
1	D	19	GLN	Peptide
1	D	60	GLU	Peptide
1	E	131	SER	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	1297	0	1386	45	0
1	B	1297	0	1386	53	0
1	C	1266	0	1353	20	1
1	D	1297	0	1386	29	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1297	0	1386	27	0
1	F	1277	0	1366	30	2
All	All	7731	0	8263	184	2

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 (184) 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:D:154:LEU:HD22	1:D:167:VAL:HG12	1.58	0.86
1:F:29:LEU:HD21	1:F:172:LEU:HD11	1.63	0.80
1:B:125:ILE:HD12	1:B:139:LEU:HD13	1.64	0.79
1:A:74:THR:HG23	1:A:76:LYS:HG2	1.65	0.79
1:A:102:THR:HG21	1:A:135:THR:HG22	1.66	0.77
1:B:87:PRO:O	1:B:88:TYR:CG	2.39	0.76
1:E:26:VAL:HG11	1:E:159:GLU:OE1	1.86	0.75
1:E:32:LEU:O	1:F:78:TYR:CZ	2.41	0.74
1:B:17:ILE:HG23	1:B:25:ALA:HB1	1.71	0.72
1:E:39:GLU:HG3	1:F:72:ARG:HD3	1.75	0.69
1:B:57:VAL:HG11	1:B:143:ILE:HD11	1.74	0.68
1:F:3:THR:HG22	1:F:14:GLU:OE1	1.95	0.67
1:F:29:LEU:HD23	1:F:129:VAL:HG21	1.78	0.66
1:A:8:ILE:HG23	1:A:169:LEU:HD21	1.79	0.65
1:A:93:VAL:HG11	1:B:28:LEU:HD13	1.79	0.64
1:D:70:LEU:O	1:D:74:THR:HB	1.98	0.64
1:D:154:LEU:CD2	1:D:167:VAL:HG12	2.28	0.63
1:A:130:VAL:HG23	1:A:155:ALA:HB2	1.81	0.62
1:E:32:LEU:HD11	1:E:62:LYS:HA	1.80	0.62
1:A:32:LEU:O	1:B:78:TYR:OH	2.16	0.61
1:E:93:VAL:HG21	1:F:18:VAL:HB	1.82	0.61
1:F:125:ILE:HB	1:F:153:VAL:HG13	1.83	0.61
1:F:24:VAL:HG23	1:F:26:VAL:CG2	2.31	0.60
1:E:89:MET:HA	1:E:94:SER:HB2	1.83	0.60
1:A:162:PRO:HB3	1:A:164:GLN:O	2.02	0.60
1:E:32:LEU:O	1:F:78:TYR:OH	2.19	0.60
1:B:70:LEU:O	1:B:74:THR:HG22	2.02	0.59
1:F:100:ILE:HG12	1:F:142:LEU:HG	1.85	0.59
1:D:154:LEU:HD22	1:D:167:VAL:CG1	2.31	0.58
1:A:112:GLY:O	1:A:115:ILE:HG23	2.04	0.57
1:A:32:LEU:HD22	1:A:62:LYS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD21	1:B:154:LEU:HD11	1.87	0.56
1:B:31:LEU:HD22	1:B:37:LEU:HD22	1.87	0.56
1:C:139:LEU:HA	1:C:142:LEU:HG	1.86	0.56
1:B:115:ILE:HB	1:B:146:VAL:HG13	1.86	0.56
1:E:3:THR:CG2	1:E:14:GLU:HB3	2.35	0.56
1:D:125:ILE:HD13	1:D:139:LEU:HD13	1.87	0.56
1:A:115:ILE:HB	1:A:146:VAL:HG13	1.89	0.55
1:A:8:ILE:HG23	1:A:169:LEU:CD2	2.37	0.55
1:B:3:THR:HG21	1:D:98:LEU:HD21	1.89	0.55
1:C:3:THR:CB	1:C:17:ILE:HG23	2.36	0.55
1:B:88:TYR:CD1	1:B:94:SER:HB2	2.42	0.55
1:E:26:VAL:HG23	1:E:174:LEU:HD13	1.89	0.55
1:E:26:VAL:CG2	1:E:174:LEU:HD13	2.36	0.54
1:E:86:LYS:O	1:E:89:MET:HB2	2.07	0.54
1:C:115:ILE:HG13	1:C:146:VAL:HG13	1.89	0.54
1:C:67:ALA:O	1:C:71:SER:OG	2.19	0.54
1:A:161:THR:OG1	1:A:162:PRO:HD2	2.07	0.53
1:A:2:ARG:NH1	1:E:97:VAL:HG12	2.21	0.53
1:B:8:ILE:HG23	1:B:169:LEU:HD23	1.91	0.53
1:A:25:ALA:HB3	1:A:175:PHE:HA	1.91	0.53
1:D:28:LEU:HD21	1:D:62:LYS:NZ	2.23	0.53
1:B:118:VAL:HB	1:B:146:VAL:HG11	1.90	0.52
1:B:88:TYR:CD1	1:B:94:SER:CB	2.92	0.52
1:B:17:ILE:CG2	1:B:25:ALA:HB1	2.39	0.52
1:A:130:VAL:HG11	1:A:166:VAL:HG21	1.92	0.52
1:C:45:LEU:HD21	1:C:155:ALA:O	2.10	0.52
1:A:32:LEU:O	1:B:78:TYR:CZ	2.62	0.51
1:A:88:TYR:HB3	1:B:18:VAL:HG21	1.92	0.51
1:B:154:LEU:HD23	1:B:167:VAL:CG1	2.40	0.51
1:B:39:GLU:OE2	1:B:72:ARG:NH1	2.44	0.51
1:A:69:ALA:O	1:A:73:ILE:HG22	2.11	0.51
1:B:6:VAL:HG22	1:B:15:LEU:HD23	1.93	0.50
1:F:3:THR:HG21	1:F:14:GLU:HB3	1.93	0.50
1:D:155:ALA:O	1:D:168:ALA:HA	2.11	0.50
1:C:157:PHE:HB3	1:C:172:LEU:CD2	2.42	0.50
1:E:3:THR:HG22	1:E:14:GLU:HB3	1.92	0.50
1:F:70:LEU:O	1:F:74:THR:HG22	2.11	0.50
1:A:130:VAL:HG23	1:A:155:ALA:CB	2.41	0.50
1:B:125:ILE:CD1	1:B:139:LEU:HD13	2.39	0.50
1:A:174:LEU:HD22	1:A:174:LEU:N	2.26	0.50
1:B:87:PRO:HA	1:B:89:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:O	1:A:73:ILE:HD12	2.11	0.50
1:D:17:ILE:CG2	1:D:25:ALA:HB1	2.41	0.50
1:D:100:ILE:HD13	1:D:141:GLU:HG3	1.93	0.49
1:E:60:GLU:OE1	1:E:82:ARG:HD3	2.11	0.49
1:E:34:ASP:OD1	1:E:37:LEU:HB2	2.12	0.49
1:D:107:LEU:HD23	1:D:108:LEU:N	2.28	0.49
1:B:167:VAL:HG13	1:B:167:VAL:O	2.12	0.49
1:D:100:ILE:HD11	1:D:142:LEU:HB2	1.93	0.49
1:D:21:GLY:O	1:D:22:PRO:C	2.49	0.49
1:A:30:ASN:HB2	1:A:62:LYS:HG3	1.94	0.48
1:A:136:LEU:HD13	1:A:164:GLN:HG3	1.95	0.48
1:D:110:LEU:HG	1:D:142:LEU:HD13	1.95	0.48
1:D:23:GLY:O	1:D:25:ALA:N	2.47	0.48
1:E:115:ILE:N	1:E:116:PRO:CD	2.77	0.48
1:B:61:VAL:CG1	1:B:64:VAL:HG22	2.44	0.48
1:C:55:VAL:HG13	1:C:123:VAL:HG22	1.96	0.48
1:D:99:SER:O	1:D:100:ILE:HG23	2.13	0.48
1:F:124:ALA:HA	1:F:152:ALA:O	2.14	0.48
1:B:34:ASP:OD2	1:D:119:ARG:NH2	2.47	0.47
1:B:105:PRO:O	1:B:106:GLN:NE2	2.47	0.47
1:B:153:VAL:HG12	1:B:166:VAL:HG13	1.94	0.47
1:B:45:LEU:CD2	1:B:169:LEU:HD13	2.44	0.47
1:C:96:GLN:HE21	1:C:96:GLN:HA	1.79	0.47
1:B:153:VAL:HG11	1:B:166:VAL:HG22	1.97	0.47
1:A:98:LEU:CD1	1:A:146:VAL:HG22	2.45	0.47
1:C:3:THR:OG1	1:C:17:ILE:HG23	2.15	0.47
1:F:100:ILE:HD11	1:F:138:GLY:O	2.15	0.46
1:F:130:VAL:HG11	1:F:166:VAL:HG21	1.98	0.46
1:B:125:ILE:HD12	1:B:139:LEU:CD1	2.42	0.46
1:A:2:ARG:HG3	1:E:96:GLN:HE21	1.80	0.46
1:B:98:LEU:HD22	1:F:3:THR:HG21	1.98	0.46
1:A:43:GLU:OE2	1:A:73:ILE:HG21	2.16	0.46
1:C:166:VAL:HG12	1:C:168:ALA:HB2	1.98	0.46
1:E:30:ASN:OD1	1:E:30:ASN:N	2.49	0.46
1:F:29:LEU:N	1:F:29:LEU:HD22	2.31	0.46
1:F:136:LEU:HD11	1:F:153:VAL:HG11	1.98	0.45
1:B:95:ARG:O	1:B:112:GLY:HA3	2.16	0.45
1:C:157:PHE:CG	1:C:172:LEU:HD21	2.51	0.45
1:A:17:ILE:HG22	1:A:25:ALA:HB1	1.99	0.45
1:A:93:VAL:HG13	1:B:16:PRO:HG2	1.98	0.45
1:A:18:VAL:HG12	1:A:26:VAL:HG21	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HD21	1:D:29:LEU:HD22	1.98	0.45
1:C:24:VAL:HG22	1:C:25:ALA:H	1.80	0.45
1:C:141:GLU:O	1:C:145:SER:OG	2.27	0.45
1:B:55:VAL:CG1	1:B:123:VAL:HG22	2.47	0.45
1:E:139:LEU:O	1:E:143:ILE:HG12	2.17	0.45
1:F:45:LEU:HD21	1:F:155:ALA:O	2.17	0.45
1:D:58:THR:HB	1:D:126:VAL:HG23	1.99	0.44
1:E:93:VAL:CG2	1:F:18:VAL:HB	2.47	0.44
1:B:8:ILE:HD11	1:B:157:PHE:CZ	2.53	0.44
1:C:18:VAL:HG11	1:D:88:TYR:CG	2.52	0.44
1:D:95:ARG:O	1:D:112:GLY:HA3	2.17	0.44
1:B:19:GLN:O	1:B:19:GLN:HG3	2.18	0.44
1:F:29:LEU:HD21	1:F:172:LEU:CD1	2.42	0.43
1:A:93:VAL:HG13	1:B:16:PRO:CG	2.48	0.43
1:A:59:PRO:O	1:A:60:GLU:O	2.35	0.43
1:D:74:THR:CG2	1:D:76:LYS:HG2	2.48	0.43
1:B:15:LEU:N	1:B:15:LEU:HD22	2.33	0.43
1:F:32:LEU:HD22	1:F:62:LYS:HB3	2.00	0.43
1:D:20:VAL:HG12	1:D:24:VAL:HG23	1.99	0.43
1:F:3:THR:CG2	1:F:14:GLU:HB3	2.49	0.43
1:F:74:THR:OG1	1:F:76:LYS:HE3	2.18	0.43
1:B:87:PRO:O	1:B:88:TYR:CD1	2.70	0.43
1:A:141:GLU:HG3	1:A:141:GLU:O	2.18	0.43
1:E:71:SER:OG	1:F:35:THR:HG21	2.19	0.43
1:B:122:LYS:HD2	1:B:151:VAL:HG11	2.01	0.43
1:C:110:LEU:HD23	1:C:111:ASP:C	2.40	0.43
1:B:95:ARG:O	1:B:96:GLN:C	2.57	0.43
1:C:171:HIS:O	1:C:172:LEU:HD13	2.19	0.43
1:A:115:ILE:N	1:A:116:PRO:CD	2.82	0.42
1:A:158:THR:HG22	1:A:170:GLY:O	2.19	0.42
1:D:38:THR:HG21	1:D:65:PRO:HB2	2.00	0.42
1:B:160:GLY:O	1:B:161:THR:HG23	2.19	0.42
1:B:64:VAL:N	1:B:65:PRO:CD	2.82	0.42
1:B:93:VAL:O	1:B:95:ARG:HG3	2.19	0.42
1:A:88:TYR:CE2	1:B:20:VAL:HG22	2.55	0.42
1:B:28:LEU:C	1:B:29:LEU:HD22	2.40	0.42
1:D:158:THR:OG1	1:D:162:PRO:HD3	2.20	0.42
1:A:89:MET:HG2	1:A:97:VAL:CG1	2.50	0.42
1:B:87:PRO:O	1:B:88:TYR:CD2	2.73	0.42
1:D:28:LEU:HD21	1:D:62:LYS:HZ3	1.85	0.42
1:F:61:VAL:HG23	1:F:62:LYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:VAL:HG13	1:E:123:VAL:HG22	2.02	0.41
1:A:95:ARG:HD2	1:A:96:GLN:N	2.35	0.41
1:A:86:LYS:O	1:A:89:MET:HB2	2.20	0.41
1:C:157:PHE:HB3	1:C:172:LEU:HD21	2.00	0.41
1:C:28:LEU:HD13	1:D:88:TYR:CE2	2.55	0.41
1:B:131:SER:O	1:B:163:ARG:NH1	2.52	0.41
1:A:162:PRO:O	1:A:163:ARG:HB3	2.21	0.41
1:A:18:VAL:HG22	1:A:19:GLN:H	1.85	0.41
1:E:111:ASP:OD1	1:E:112:GLY:N	2.53	0.41
1:B:60:GLU:CG	1:B:82:ARG:HA	2.50	0.41
1:A:159:GLU:HG3	1:A:159:GLU:O	2.20	0.41
1:B:153:VAL:O	1:B:167:VAL:HG12	2.20	0.41
1:E:6:VAL:HG22	1:E:13:ARG:O	2.21	0.41
1:A:164:GLN:O	1:A:166:VAL:HG23	2.20	0.41
1:F:43:GLU:OE2	1:F:43:GLU:CA	2.69	0.41
1:A:18:VAL:HG22	1:A:19:GLN:N	2.35	0.41
1:D:17:ILE:HG23	1:D:25:ALA:HB1	2.03	0.41
1:E:57:VAL:HG11	1:E:143:ILE:HD11	2.02	0.41
1:E:59:PRO:HA	1:E:81:ALA:O	2.21	0.41
1:A:136:LEU:HD13	1:A:164:GLN:CG	2.51	0.41
1:A:18:VAL:HG12	1:A:26:VAL:CG2	2.51	0.40
1:F:115:ILE:N	1:F:116:PRO:CD	2.84	0.40
1:F:100:ILE:HD11	1:F:142:LEU:HB2	2.04	0.40
1:B:114:ASP:HA	1:B:117:ARG:HD2	2.03	0.40
1:B:146:VAL:O	1:B:146:VAL:HG12	2.21	0.40
1:E:64:VAL:N	1:E:65:PRO:HD2	2.35	0.40
1:F:15:LEU:HD21	1:F:29:LEU:CD1	2.51	0.40
1:D:128:ASP:OD1	1:D:129:VAL:N	2.55	0.40
1:C:24:VAL:HG13	1:C:25:ALA:N	2.36	0.40
1:C:15:LEU:HD12	1:C:28:LEU:O	2.22	0.40

All (2) 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)
1:C:89:MET:O	1:F:119:ARG:NH2[1_654]	2.08	0.12
1:D:169:LEU:O	1:F:7:GLU:OE2[2_848]	2.13	0.07

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	172/174 (99%)	141 (82%)	20 (12%)	11 (6%)	1 2
1	B	172/174 (99%)	147 (86%)	19 (11%)	6 (4%)	3 8
1	C	169/174 (97%)	136 (80%)	23 (14%)	10 (6%)	1 2
1	D	172/174 (99%)	148 (86%)	18 (10%)	6 (4%)	3 8
1	E	172/174 (99%)	147 (86%)	20 (12%)	5 (3%)	4 10
1	F	170/174 (98%)	147 (86%)	20 (12%)	3 (2%)	8 21
All	All	1027/1044 (98%)	866 (84%)	120 (12%)	41 (4%)	3 6

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ALA
1	A	32	LEU
1	A	60	GLU
1	A	93	VAL
1	B	24	VAL
1	B	89	MET
1	C	61	VAL
1	C	93	VAL
1	D	32	LEU
1	E	61	VAL
1	E	93	VAL
1	F	51	PRO
1	F	61	VAL
1	B	105	PRO
1	C	24	VAL
1	E	24	VAL
1	E	131	SER
1	F	93	VAL
1	A	162	PRO
1	A	163	ARG

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Mol	Chain	Res	Type
1	B	88	TYR
1	C	147	GLY
1	D	24	VAL
1	A	61	VAL
1	B	163	ARG
1	C	11	VAL
1	A	85	GLU
1	C	146	VAL
1	D	105	PRO
1	D	133	GLY
1	A	131	SER
1	C	119	ARG
1	B	22	PRO
1	E	150	VAL
1	A	26	VAL
1	C	59	PRO
1	C	97	VAL
1	C	112	GLY
1	D	61	VAL
1	D	103	GLY
1	A	160	GLY

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	142/142 (100%)	112 (79%)	30 (21%)	1	3
1	B	142/142 (100%)	118 (83%)	24 (17%)	2	5
1	C	139/142 (98%)	114 (82%)	25 (18%)	1	4
1	D	142/142 (100%)	107 (75%)	35 (25%)	0	2
1	E	142/142 (100%)	118 (83%)	24 (17%)	2	5
1	F	140/142 (99%)	106 (76%)	34 (24%)	0	2
All	All	847/852 (99%)	675 (80%)	172 (20%)	1	3

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	12	ARG
1	A	19	GLN
1	A	31	LEU
1	A	32	LEU
1	A	37	LEU
1	A	39	GLU
1	A	43	GLU
1	A	47	LYS
1	A	48	ARG
1	A	49	LEU
1	A	62	LYS
1	A	70	LEU
1	A	71	SER
1	A	74	THR
1	A	89	MET
1	A	95	ARG
1	A	102	THR
1	A	104	LYS
1	A	109	VAL
1	A	115	ILE
1	A	132	THR
1	A	136	LEU
1	A	139	LEU
1	A	145	SER
1	A	159	GLU
1	A	161	THR
1	A	164	GLN
1	A	174	LEU
1	A	175	PHE
1	B	39	GLU
1	B	47	LYS
1	B	48	ARG
1	B	49	LEU
1	B	61	VAL
1	B	66	LEU
1	B	71	SER
1	B	85	GLU
1	B	88	TYR
1	B	89	MET
1	B	95	ARG
1	B	96	GLN

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Mol	Chain	Res	Type
1	B	106	GLN
1	B	109	VAL
1	B	115	ILE
1	B	117	ARG
1	B	126	VAL
1	B	136	LEU
1	B	139	LEU
1	B	140	ARG
1	B	142	LEU
1	B	145	SER
1	B	161	THR
1	B	174	LEU
1	C	3	THR
1	C	7	GLU
1	C	12	ARG
1	C	15	LEU
1	C	17	ILE
1	C	32	LEU
1	C	37	LEU
1	C	48	ARG
1	C	66	LEU
1	C	76	LYS
1	C	89	MET
1	C	90	ILE
1	C	93	VAL
1	C	95	ARG
1	C	96	GLN
1	C	99	SER
1	C	100	ILE
1	C	102	THR
1	C	106	GLN
1	C	107	LEU
1	C	111	ASP
1	C	117	ARG
1	C	141	GLU
1	C	163	ARG
1	C	172	LEU
1	D	2	ARG
1	D	3	THR
1	D	7	GLU
1	D	28	LEU
1	D	29	LEU

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Mol	Chain	Res	Type
1	D	31	LEU
1	D	32	LEU
1	D	37	LEU
1	D	47	LYS
1	D	49	LEU
1	D	61	VAL
1	D	62	LYS
1	D	71	SER
1	D	74	THR
1	D	76	LYS
1	D	89	MET
1	D	96	GLN
1	D	100	ILE
1	D	101	THR
1	D	109	VAL
1	D	110	LEU
1	D	125	ILE
1	D	132	THR
1	D	136	LEU
1	D	139	LEU
1	D	140	ARG
1	D	142	LEU
1	D	146	VAL
1	D	154	LEU
1	D	158	THR
1	D	163	ARG
1	D	164	GLN
1	D	165	ASP
1	D	167	VAL
1	D	174	LEU
1	E	30	ASN
1	E	31	LEU
1	E	37	LEU
1	E	52	GLU
1	E	66	LEU
1	E	72	ARG
1	E	74	THR
1	E	76	LYS
1	E	85	GLU
1	E	88	TYR
1	E	89	MET
1	E	93	VAL

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Mol	Chain	Res	Type
1	E	96	GLN
1	E	99	SER
1	E	108	LEU
1	E	115	ILE
1	E	117	ARG
1	E	134	SER
1	E	136	LEU
1	E	140	ARG
1	E	141	GLU
1	E	161	THR
1	E	163	ARG
1	E	174	LEU
1	F	2	ARG
1	F	15	LEU
1	F	31	LEU
1	F	32	LEU
1	F	37	LEU
1	F	43	GLU
1	F	47	LYS
1	F	48	ARG
1	F	49	LEU
1	F	51	PRO
1	F	62	LYS
1	F	64	VAL
1	F	66	LEU
1	F	85	GLU
1	F	86	LYS
1	F	89	MET
1	F	93	VAL
1	F	95	ARG
1	F	98	LEU
1	F	107	LEU
1	F	115	ILE
1	F	117	ARG
1	F	119	ARG
1	F	122	LYS
1	F	134	SER
1	F	136	LEU
1	F	139	LEU
1	F	141	GLU
1	F	142	LEU
1	F	154	LEU

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Mol	Chain	Res	Type
1	F	158	THR
1	F	161	THR
1	F	163	ARG
1	F	167	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	B	68	HIS
1	C	68	HIS
1	C	96	GLN
1	C	164	GLN
1	D	164	GLN
1	E	68	HIS
1	E	96	GLN
1	F	68	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	174/174 (100%)	0.62	17 (9%) 7 5	25, 39, 77, 123	0
1	B	174/174 (100%)	0.65	23 (13%) 3 2	19, 34, 85, 99	0
1	C	171/174 (98%)	1.53	50 (29%) 0 0	21, 59, 104, 135	0
1	D	174/174 (100%)	0.74	23 (13%) 3 2	14, 30, 73, 122	0
1	E	174/174 (100%)	1.12	37 (21%) 0 0	19, 45, 96, 123	0
1	F	172/174 (98%)	0.78	28 (16%) 1 1	16, 38, 83, 119	0
All	All	1039/1044 (99%)	0.91	178 (17%) 1 1	14, 40, 94, 135	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	PRO	23.4
1	D	91	ASN	11.8
1	A	90	ILE	11.2
1	E	163	ARG	11.0
1	E	92	PRO	10.2
1	D	93	VAL	10.1
1	D	88	TYR	9.1
1	B	24	VAL	8.6
1	C	90	ILE	8.2
1	F	88	TYR	8.2
1	C	91	ASN	8.2
1	E	93	VAL	8.1
1	C	93	VAL	7.7
1	A	91	ASN	7.6
1	A	88	TYR	7.1
1	F	89	MET	7.1
1	D	92	PRO	6.9
1	C	109	VAL	6.7
1	F	162	PRO	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	25	ALA	6.6
1	C	103	GLY	6.5
1	D	162	PRO	6.3
1	D	90	ILE	5.9
1	E	175	PHE	5.9
1	E	104	LYS	5.9
1	B	93	VAL	5.8
1	C	97	VAL	5.7
1	A	92	PRO	5.5
1	D	89	MET	5.5
1	F	92	PRO	5.3
1	B	92	PRO	5.2
1	E	90	ILE	5.2
1	C	108	LEU	5.2
1	F	164	GLN	5.2
1	F	93	VAL	5.1
1	E	164	GLN	5.0
1	D	175	PHE	4.9
1	F	90	ILE	4.8
1	F	18	VAL	4.8
1	A	93	VAL	4.8
1	B	105	PRO	4.8
1	B	89	MET	4.7
1	D	163	ARG	4.5
1	D	24	VAL	4.5
1	D	106	GLN	4.5
1	F	22	PRO	4.5
1	B	164	GLN	4.5
1	C	163	ARG	4.4
1	D	20	VAL	4.4
1	E	134	SER	4.4
1	F	87	PRO	4.4
1	A	133	GLY	4.3
1	C	94	SER	4.3
1	E	162	PRO	4.2
1	E	105	PRO	4.2
1	B	163	ARG	4.2
1	D	105	PRO	4.2
1	C	104	LYS	4.2
1	C	106	GLN	4.2
1	C	20	VAL	4.1
1	E	87	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	89	MET	4.0
1	F	105	PRO	4.0
1	B	90	ILE	4.0
1	E	95	ARG	3.9
1	E	165	ASP	3.9
1	B	22	PRO	3.9
1	E	106	GLN	3.9
1	D	94	SER	3.9
1	C	117	ARG	3.9
1	F	26	VAL	3.8
1	B	87	PRO	3.8
1	C	160	GLY	3.7
1	C	96	GLN	3.7
1	B	61	VAL	3.7
1	E	103	GLY	3.6
1	E	174	LEU	3.6
1	A	89	MET	3.6
1	C	86	LYS	3.6
1	F	24	VAL	3.6
1	F	134	SER	3.6
1	A	159	GLU	3.6
1	B	94	SER	3.5
1	F	95	ARG	3.5
1	F	161	THR	3.4
1	B	23	GLY	3.4
1	D	95	ARG	3.3
1	C	26	VAL	3.3
1	C	87	PRO	3.3
1	C	151	VAL	3.2
1	A	87	PRO	3.2
1	C	99	SER	3.2
1	F	72	ARG	3.2
1	E	25	ALA	3.1
1	F	20	VAL	3.1
1	E	88	TYR	3.1
1	C	146	VAL	3.1
1	B	175	PHE	3.1
1	C	132	THR	3.1
1	C	149	GLU	3.0
1	E	89	MET	3.0
1	F	84	THR	3.0
1	C	161	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	24	VAL	3.0
1	E	107	LEU	3.0
1	C	107	LEU	2.9
1	C	105	PRO	2.9
1	A	99	SER	2.9
1	E	26	VAL	2.9
1	B	91	ASN	2.8
1	C	88	TYR	2.8
1	B	20	VAL	2.8
1	A	94	SER	2.8
1	E	91	ASN	2.8
1	D	21	GLY	2.8
1	E	19	GLN	2.7
1	F	165	ASP	2.7
1	F	103	GLY	2.7
1	D	104	LYS	2.7
1	B	21	GLY	2.7
1	F	94	SER	2.6
1	C	158	THR	2.6
1	B	2	ARG	2.6
1	E	52	GLU	2.6
1	C	95	ARG	2.6
1	C	166	VAL	2.6
1	C	110	LEU	2.6
1	C	133	GLY	2.6
1	E	101	THR	2.6
1	C	98	LEU	2.6
1	F	91	ASN	2.5
1	E	132	THR	2.5
1	A	164	GLN	2.5
1	C	162	PRO	2.5
1	A	132	THR	2.5
1	B	18	VAL	2.5
1	A	21	GLY	2.4
1	C	84	THR	2.4
1	D	73	ILE	2.4
1	E	133	GLY	2.4
1	D	25	ALA	2.3
1	E	61	VAL	2.3
1	F	133	GLY	2.3
1	E	135	THR	2.3
1	F	163	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	162	PRO	2.3
1	B	132	THR	2.3
1	D	101	THR	2.3
1	A	161	THR	2.3
1	C	120	GLY	2.2
1	C	171	HIS	2.2
1	B	161	THR	2.2
1	D	97	VAL	2.2
1	D	85	GLU	2.2
1	F	96	GLN	2.2
1	C	23	GLY	2.2
1	E	161	THR	2.2
1	E	51	PRO	2.2
1	E	23	GLY	2.2
1	E	102	THR	2.1
1	C	83	LYS	2.1
1	E	144	GLU	2.1
1	C	102	THR	2.1
1	C	101	THR	2.1
1	C	165	ASP	2.1
1	C	100	ILE	2.1
1	C	60	GLU	2.1
1	A	146	VAL	2.1
1	F	104	LYS	2.1
1	A	51	PRO	2.1
1	C	19	GLN	2.1
1	E	8	ILE	2.0
1	B	174	LEU	2.0
1	C	52	GLU	2.0
1	C	57	VAL	2.0
1	F	149	GLU	2.0
1	D	164	GLN	2.0
1	E	94	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.