Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:20 PM JST

PDB ID	:	5Y6O
Title	:	Crystal structure of DAXX N-terminal four-helix bundle domain (4HB) in complex with ATRX
Authors	:	Huang, H.; Patel, D.J.
Deposited on	:	2017-08-13
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

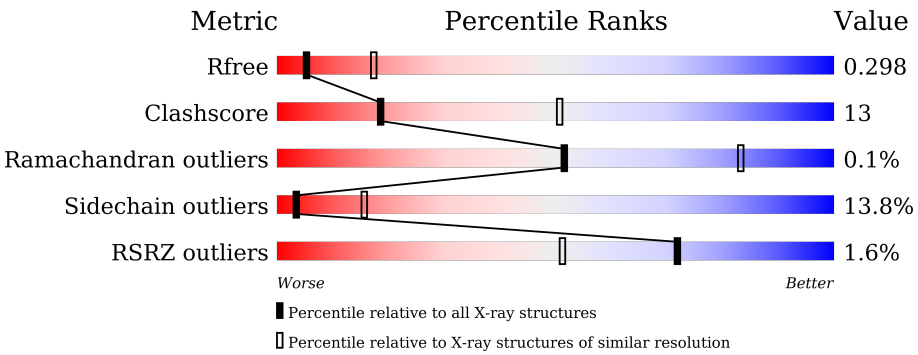
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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% 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	119	3%, 63%, 23%, •, 12%
1	B	119	%, 57%, 28%, •, 12%
1	C	119	%, 49%, 36%, •, 11%
1	D	119	3%, 63%, 23%, 5%, 9%
1	E	119	62%, 21%, 8%, 9%
1	F	119	2%, 55%, 29%, •, 13%

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Mol	Chain	Length	Quality of chain
1	G	119	3% 55% 27% 6% 12%
1	H	119	56% 23% 8% 13%
1	I	119	2% 56% 25% 5% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7467 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 Death domain-associated protein 6,Transcriptional regulator ATRX.

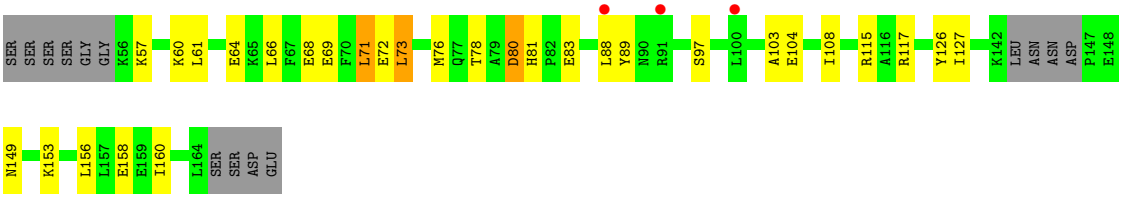
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	105	826	530	140	150	6	0	0	0
1	B	105	827	528	145	148	6	0	0	0
1	C	106	827	529	145	147	6	0	0	0
1	D	108	826	529	139	152	6	0	0	0
1	E	108	840	537	145	152	6	0	0	0
1	F	104	835	531	147	151	6	0	0	0
1	G	105	835	533	145	151	6	0	0	0
1	H	103	815	522	139	148	6	0	0	0
1	I	103	836	532	147	151	6	0	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 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.

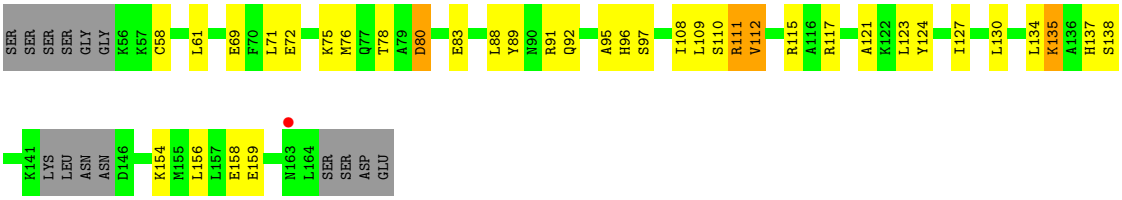
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain A:



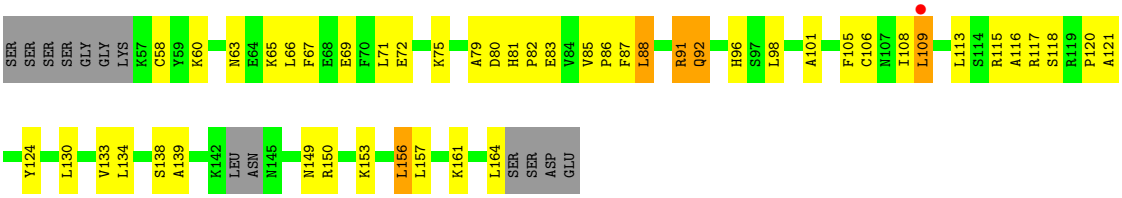
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain B:



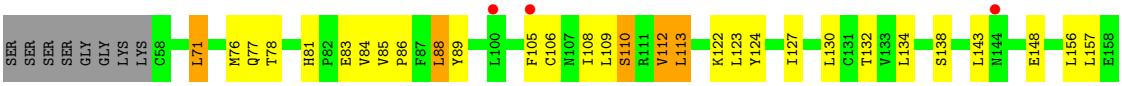
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

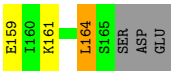
Chain C:



• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

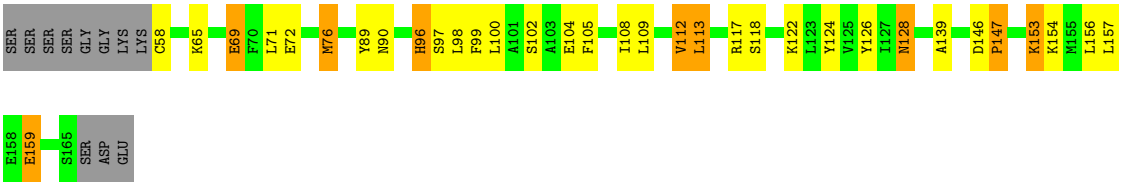
Chain D:





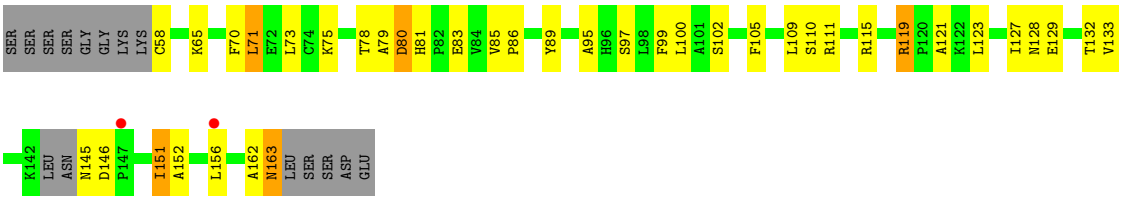
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain E:



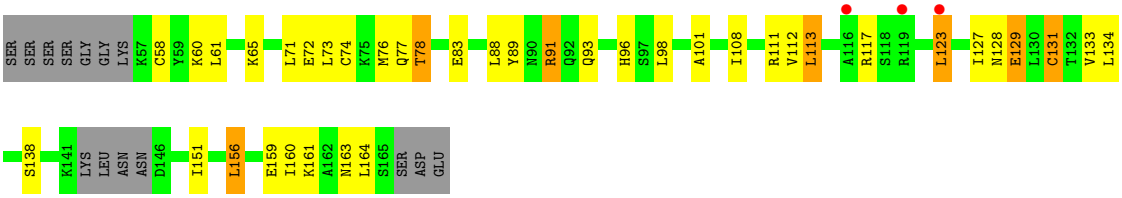
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain F:



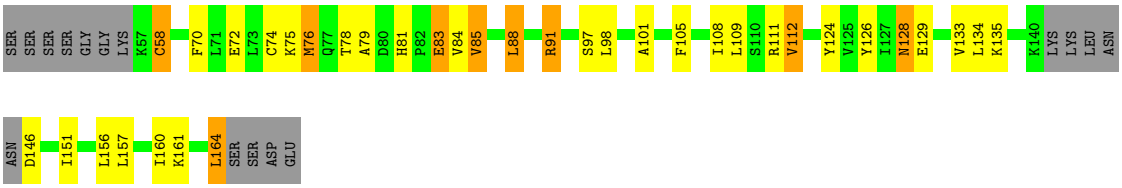
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain G:



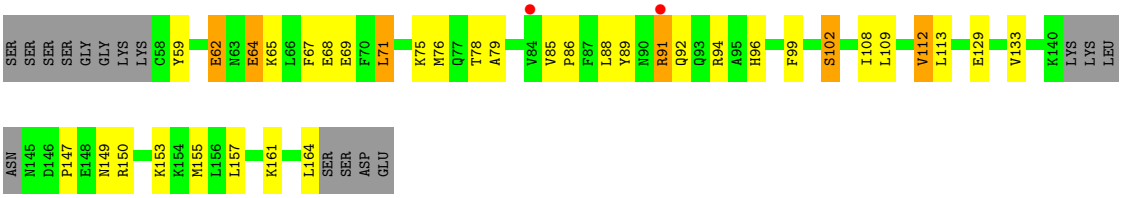
• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain H:



• Molecule 1: Death domain-associated protein 6,Transcriptional regulator ATRX

Chain I:


SER SER SER SER GLY GLY LYS LYS C58 Y59 E62 N63 E64 K65 L66 F67 E68 E69 F70 L71 K75 M76 Q77 T78 A79 V84 V85 P86 F87 L88 Y89 N90 R91 Q92 Q93 R94 A95 H96 F99 S102 I108 L109 V112 L113 E129 V133 K140 LYS LYS LEU

ASN N145 D146 P147 E148 N149 R150 K153 K154 M155 L156 L157 K161 L164 SER SER ASP GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.67Å 78.67Å 503.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.87 – 3.10 83.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (83.87-3.10) 94.0 (83.87-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.224 , 0.297 0.225 , 0.298	Depositor DCC
R_{free} test set	1731 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	101.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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 (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	0.45	0/840	0.66	0/1132
1	B	0.54	0/841	0.70	0/1134
1	C	0.50	0/841	0.72	1/1136 (0.1%)
1	D	0.45	0/841	0.67	0/1140
1	E	0.46	0/855	0.67	0/1156
1	F	0.50	0/849	0.72	0/1143
1	G	0.44	0/849	0.68	0/1144
1	H	0.52	0/829	0.70	0/1119
1	I	0.44	0/850	0.66	0/1144
All	All	0.48	0/7595	0.69	1/10248 (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
1	C	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	156	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	138	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	139	ALA	Peptide
1	D	143	LEU	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	826	0	817	26	0
1	B	827	0	814	21	0
1	C	827	0	810	31	0
1	D	826	0	796	26	0
1	E	840	0	822	26	0
1	F	835	0	829	25	0
1	G	835	0	830	25	0
1	H	815	0	803	29	0
1	I	836	0	840	19	0
All	All	7467	0	7361	195	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 13.

All (195) 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:H:91:ARG:HG2	1:H:91:ARG:HH11	1.25	1.02
1:B:91:ARG:HE	1:B:135:LYS:HG2	1.41	0.85
1:A:88:LEU:HD11	1:A:127:ILE:HG23	1.60	0.83
1:G:91:ARG:HG2	1:G:91:ARG:HH11	1.43	0.82
1:C:91:ARG:HG2	1:C:91:ARG:HH11	1.50	0.77
1:E:58:CYS:HB3	1:H:58:CYS:HB3	1.69	0.74
1:A:57:LYS:HD2	1:A:103:ALA:H	1.52	0.74
1:A:149:ASN:ND2	1:C:121:ALA:O	2.22	0.73
1:H:91:ARG:HG2	1:H:91:ARG:NH1	1.98	0.72
1:G:78:THR:OG1	1:G:78:THR:O	2.04	0.71
1:C:69:GLU:OE1	1:C:117:ARG:NH2	2.24	0.70
1:F:58:CYS:HB3	1:G:58:CYS:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:HA	1:C:118:SER:HB3	1.74	0.69
1:A:69:GLU:OE1	1:A:117:ARG:NH2	2.24	0.68
1:E:96:HIS:CE1	1:E:139:ALA:HB2	2.30	0.67
1:G:91:ARG:HG2	1:G:91:ARG:NH1	2.09	0.67
1:D:122:LYS:HZ3	1:E:147:PRO:HB2	1.59	0.67
1:A:80:ASP:OD2	1:A:81:HIS:ND1	2.29	0.66
1:F:111:ARG:NH2	1:F:129:GLU:OE1	2.29	0.66
1:A:78:THR:O	1:A:78:THR:OG1	2.13	0.64
1:H:112:VAL:HG23	1:H:126:TYR:HB3	1.80	0.64
1:C:92:GLN:HA	1:C:134:LEU:HD22	1.79	0.63
1:E:72:GLU:OE2	1:F:75:LYS:NZ	2.29	0.63
1:E:76:MET:HG3	1:F:89:TYR:CG	2.34	0.63
1:B:111:ARG:HD3	1:B:115:ARG:HE	1.65	0.62
1:B:80:ASP:N	1:B:80:ASP:OD1	2.33	0.61
1:D:81:HIS:HB3	1:D:83:GLU:OE2	2.00	0.61
1:I:108:ILE:O	1:I:112:VAL:HG13	2.01	0.61
1:A:60:LYS:HG2	1:A:61:LEU:HD23	1.84	0.60
1:A:81:HIS:HB3	1:A:83:GLU:OE2	2.02	0.60
1:E:122:LYS:NZ	1:F:146:ASP:OD1	2.26	0.60
1:A:60:LYS:HE3	1:A:64:GLU:OE2	2.02	0.60
1:B:91:ARG:NE	1:B:135:LYS:HG2	2.15	0.59
1:C:87:PHE:CE1	1:C:91:ARG:NH1	2.71	0.58
1:B:78:THR:O	1:B:78:THR:OG1	2.18	0.58
1:F:162:ALA:HA	1:F:163:ASN:C	2.24	0.58
1:A:72:GLU:OE2	1:B:75:LYS:NZ	2.36	0.57
1:F:85:VAL:HB	1:F:86:PRO:HD3	1.86	0.57
1:B:91:ARG:HH11	1:B:91:ARG:HG2	1.69	0.57
1:D:109:LEU:O	1:D:113:LEU:HB2	2.05	0.57
1:C:60:LYS:HB2	1:C:101:ALA:HB2	1.87	0.57
1:A:71:LEU:HG	1:A:89:TYR:CE2	2.39	0.56
1:D:89:TYR:CD1	1:F:79:ALA:HB3	2.40	0.56
1:A:115:ARG:HB3	1:A:126:TYR:CZ	2.40	0.56
1:H:129:GLU:O	1:H:133:VAL:HG23	2.05	0.56
1:G:156:LEU:O	1:G:160:ILE:HG13	2.05	0.56
1:C:91:ARG:HH11	1:C:91:ARG:CG	2.17	0.55
1:G:108:ILE:HD13	1:G:133:VAL:HG11	1.89	0.55
1:E:108:ILE:O	1:E:112:VAL:HG12	2.06	0.55
1:H:108:ILE:O	1:H:112:VAL:HG12	2.07	0.55
1:D:76:MET:HB3	1:E:89:TYR:CD1	2.42	0.54
1:D:78:THR:O	1:D:78:THR:OG1	2.19	0.54
1:B:69:GLU:OE2	1:B:117:ARG:NH2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ASP:N	1:E:147:PRO:HD2	2.23	0.54
1:G:113:LEU:O	1:G:117:ARG:HD2	2.08	0.54
1:H:78:THR:HG21	1:H:84:VAL:HB	1.90	0.54
1:D:88:LEU:HD21	1:D:130:LEU:HD23	1.90	0.53
1:F:123:LEU:HG	1:F:127:ILE:HD11	1.91	0.53
1:C:82:PRO:HD2	1:C:83:GLU:OE2	2.09	0.53
1:F:78:THR:O	1:F:78:THR:OG1	2.17	0.53
1:G:159:GLU:O	1:G:163:ASN:ND2	2.28	0.53
1:D:123:LEU:O	1:D:127:ILE:HG13	2.08	0.52
1:G:131:CYS:HA	1:G:134:LEU:HB2	1.90	0.52
1:C:153:LYS:HG2	1:C:157:LEU:HD12	1.90	0.52
1:A:66:LEU:HA	1:A:69:GLU:HG3	1.91	0.52
1:A:60:LYS:O	1:A:64:GLU:HG3	2.09	0.52
1:E:69:GLU:OE1	1:E:117:ARG:NH2	2.43	0.52
1:A:160:ILE:HG21	1:C:83:GLU:HB3	1.91	0.52
1:I:65:LYS:O	1:I:69:GLU:HG3	2.10	0.52
1:D:122:LYS:HZ3	1:E:147:PRO:CB	2.23	0.51
1:A:104:GLU:O	1:A:108:ILE:HG13	2.09	0.51
1:G:89:TYR:CD2	1:I:79:ALA:HB3	2.45	0.51
1:F:128:ASN:O	1:F:132:THR:HG23	2.10	0.51
1:G:161:LYS:O	1:G:164:LEU:HB2	2.10	0.51
1:B:130:LEU:O	1:B:134:LEU:HB2	2.10	0.51
1:C:67:PHE:HB2	1:C:109:LEU:HD11	1.93	0.51
1:D:105:PHE:HA	1:D:108:ILE:HD12	1.92	0.51
1:F:70:PHE:O	1:F:73:LEU:HB3	2.10	0.51
1:A:153:LYS:HE2	1:C:124:TYR:CE2	2.46	0.50
1:H:124:TYR:O	1:H:128:ASN:HB2	2.12	0.50
1:E:113:LEU:O	1:E:117:ARG:HG3	2.11	0.50
1:A:156:LEU:O	1:A:160:ILE:HG12	2.12	0.50
1:D:106:CYS:O	1:D:110:SER:OG	2.29	0.50
1:E:105:PHE:CE2	1:E:109:LEU:HD11	2.47	0.49
1:D:124:TYR:CE2	1:E:153:LYS:HD3	2.48	0.49
1:B:92:GLN:O	1:B:95:ALA:HB3	2.13	0.48
1:H:79:ALA:HB2	1:I:86:PRO:HB2	1.95	0.48
1:H:108:ILE:HD13	1:H:133:VAL:HG11	1.95	0.48
1:G:74:CYS:C	1:G:76:MET:H	2.17	0.48
1:C:72:GLU:HA	1:C:75:LYS:HG3	1.94	0.48
1:G:60:LYS:HB2	1:G:101:ALA:HB2	1.94	0.48
1:A:66:LEU:HD23	1:A:69:GLU:HG3	1.96	0.48
1:A:68:GLU:OE2	1:C:79:ALA:HB3	2.13	0.48
1:I:91:ARG:HH22	1:I:94:ARG:NH1	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:GLU:OE2	1:I:75:LYS:NZ	2.47	0.48
1:B:72:GLU:O	1:B:72:GLU:HG3	2.13	0.48
1:A:115:ARG:HD3	1:A:126:TYR:CE1	2.48	0.47
1:B:121:ALA:O	1:C:149:ASN:ND2	2.47	0.47
1:C:75:LYS:O	1:C:79:ALA:HB2	2.14	0.47
1:D:77:GLN:NE2	1:E:90:ASN:OD1	2.31	0.47
1:G:77:GLN:HG3	1:G:123:LEU:HD13	1.96	0.47
1:E:124:TYR:O	1:E:128:ASN:HB2	2.14	0.47
1:B:95:ALA:HA	1:B:137:HIS:O	2.15	0.47
1:C:81:HIS:HB3	1:C:83:GLU:OE1	2.15	0.47
1:F:119:ARG:HH11	1:F:121:ALA:HB3	1.80	0.47
1:D:81:HIS:CE1	1:E:157:LEU:HD11	2.49	0.47
1:E:112:VAL:HG23	1:E:126:TYR:HB3	1.97	0.46
1:I:91:ARG:HH22	1:I:94:ARG:HH11	1.62	0.46
1:D:89:TYR:CE2	1:F:80:ASP:OD2	2.68	0.46
1:H:81:HIS:O	1:H:83:GLU:N	2.43	0.46
1:B:135:LYS:O	1:B:138:SER:OG	2.34	0.46
1:H:75:LYS:HG2	1:H:85:VAL:HG11	1.98	0.46
1:I:99:PHE:O	1:I:102:SER:HB3	2.15	0.46
1:D:86:PRO:HB3	1:F:80:ASP:HA	1.97	0.46
1:C:88:LEU:HD21	1:C:130:LEU:HD23	1.98	0.46
1:D:122:LYS:NZ	1:E:147:PRO:HB2	2.29	0.46
1:F:99:PHE:HA	1:F:102:SER:HB3	1.98	0.46
1:A:88:LEU:HA	1:A:88:LEU:HD23	1.70	0.46
1:D:108:ILE:O	1:D:112:VAL:HG13	2.16	0.45
1:E:102:SER:OG	1:E:104:GLU:HB3	2.15	0.45
1:F:129:GLU:O	1:F:133:VAL:HG23	2.16	0.45
1:I:153:LYS:HG3	1:I:157:LEU:HD12	1.97	0.45
1:F:71:LEU:O	1:F:75:LYS:HG3	2.16	0.45
1:H:156:LEU:O	1:H:160:ILE:HG13	2.17	0.45
1:H:74:CYS:O	1:H:78:THR:HB	2.16	0.45
1:I:129:GLU:O	1:I:133:VAL:HG23	2.16	0.45
1:H:76:MET:HA	1:I:86:PRO:HB3	1.99	0.45
1:I:147:PRO:O	1:I:149:ASN:N	2.50	0.45
1:C:87:PHE:CZ	1:C:91:ARG:NH1	2.85	0.45
1:D:161:LYS:O	1:D:164:LEU:HB2	2.16	0.45
1:E:99:PHE:HA	1:E:102:SER:HB2	1.99	0.45
1:G:123:LEU:HD21	1:G:127:ILE:HD11	1.99	0.45
1:H:161:LYS:O	1:H:164:LEU:HB2	2.16	0.45
1:C:98:LEU:O	1:C:101:ALA:N	2.43	0.44
1:H:91:ARG:NE	1:H:135:LYS:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:LEU:O	1:I:113:LEU:HB2	2.16	0.44
1:F:105:PHE:CZ	1:F:109:LEU:HD11	2.52	0.44
1:C:83:GLU:H	1:C:83:GLU:CD	2.21	0.44
1:H:70:PHE:HE1	1:H:88:LEU:HD11	1.83	0.44
1:E:159:GLU:O	1:E:159:GLU:HG3	2.17	0.44
1:B:76:MET:HA	1:C:86:PRO:HB3	2.00	0.43
1:H:157:LEU:HD23	1:H:157:LEU:HA	1.77	0.43
1:C:66:LEU:HD23	1:C:113:LEU:HD12	1.99	0.43
1:G:108:ILE:O	1:G:112:VAL:HG13	2.17	0.43
1:F:145:ASN:HA	1:F:146:ASP:HA	1.62	0.43
1:B:124:TYR:HB2	1:C:149:ASN:OD1	2.19	0.43
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.54	0.43
1:D:71:LEU:HD13	1:D:85:VAL:HG13	2.00	0.43
1:D:122:LYS:NZ	1:E:147:PRO:CB	2.82	0.43
1:I:64:GLU:O	1:I:68:GLU:HG3	2.18	0.43
1:B:108:ILE:O	1:B:112:VAL:HG12	2.19	0.43
1:C:63:ASN:OD1	1:C:106:CYS:HA	2.19	0.42
1:C:75:LYS:HG2	1:C:85:VAL:HG11	2.01	0.42
1:C:161:LYS:O	1:C:164:LEU:HB2	2.19	0.42
1:C:65:LYS:O	1:C:69:GLU:HG3	2.19	0.42
1:D:81:HIS:O	1:D:84:VAL:HG23	2.19	0.42
1:H:105:PHE:CZ	1:H:134:LEU:HD21	2.55	0.42
1:I:59:TYR:O	1:I:62:GLU:HG2	2.19	0.42
1:D:157:LEU:HD23	1:D:157:LEU:HA	1.79	0.42
1:H:76:MET:HG3	1:I:89:TYR:CG	2.54	0.42
1:H:78:THR:O	1:H:78:THR:CG2	2.67	0.42
1:A:115:ARG:HB3	1:A:126:TYR:CE1	2.54	0.42
1:F:81:HIS:HB3	1:F:83:GLU:OE1	2.20	0.42
1:G:72:GLU:OE2	1:H:75:LYS:NZ	2.51	0.42
1:D:81:HIS:HE1	1:E:153:LYS:NZ	2.17	0.42
1:F:95:ALA:HB3	1:F:100:LEU:HD11	2.02	0.42
1:H:78:THR:O	1:H:78:THR:HG22	2.19	0.42
1:G:73:LEU:C	1:G:74:CYS:O	2.58	0.42
1:C:116:ALA:O	1:C:120:PRO:HB3	2.19	0.42
1:G:93:GLN:H	1:G:93:GLN:HG2	1.57	0.42
1:H:81:HIS:O	1:H:84:VAL:HG23	2.20	0.42
1:B:109:LEU:HA	1:B:112:VAL:HG13	2.01	0.42
1:D:156:LEU:O	1:D:159:GLU:HB3	2.19	0.42
1:I:161:LYS:HA	1:I:164:LEU:HD12	2.02	0.42
1:F:151:ILE:HG22	1:F:152:ALA:N	2.35	0.41
1:B:91:ARG:HG2	1:B:91:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:LYS:HB2	1:H:135:LYS:HE2	1.78	0.41
1:G:73:LEU:HA	1:G:73:LEU:HD12	1.80	0.41
1:E:96:HIS:HE1	1:E:139:ALA:HB2	1.82	0.41
1:G:129:GLU:H	1:G:129:GLU:HG2	1.65	0.41
1:B:123:LEU:O	1:B:127:ILE:HG13	2.21	0.41
1:G:71:LEU:HD23	1:G:71:LEU:HA	1.83	0.41
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.80	0.41
1:C:105:PHE:HA	1:C:108:ILE:HD12	2.02	0.40
1:G:83:GLU:OE1	1:G:83:GLU:N	2.38	0.40
1:G:123:LEU:O	1:G:127:ILE:HG13	2.20	0.40
1:A:66:LEU:HA	1:A:69:GLU:CG	2.51	0.40
1:E:98:LEU:C	1:E:100:LEU:H	2.24	0.40
1:F:58:CYS:HB3	1:G:58:CYS:CB	2.47	0.40
1:I:67:PHE:CE2	1:I:71:LEU:HG	2.56	0.40
1:A:76:MET:HB3	1:B:89:TYR:CD1	2.56	0.40
1:H:98:LEU:O	1:H:101:ALA:N	2.47	0.40
1:F:119:ARG:NH1	1:F:121:ALA:HB3	2.36	0.40
1:I:78:THR:O	1:I:78:THR:OG1	2.15	0.40
1:H:91:ARG:HH11	1:H:91:ARG:CG	2.11	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	101/119 (85%)	95 (94%)	6 (6%)	0	100 100
1	B	101/119 (85%)	94 (93%)	7 (7%)	0	100 100
1	C	102/119 (86%)	89 (87%)	13 (13%)	0	100 100
1	D	106/119 (89%)	94 (89%)	12 (11%)	0	100 100
1	E	106/119 (89%)	88 (83%)	17 (16%)	1 (1%)	17 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	100/119 (84%)	91 (91%)	9 (9%)	0	100	100
1	G	101/119 (85%)	92 (91%)	9 (9%)	0	100	100
1	H	99/119 (83%)	91 (92%)	8 (8%)	0	100	100
1	I	99/119 (83%)	91 (92%)	8 (8%)	0	100	100
All	All	915/1071 (85%)	825 (90%)	89 (10%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	147	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	87/107 (81%)	82 (94%)	5 (6%)	20	52
1	B	86/107 (80%)	70 (81%)	16 (19%)	1	7
1	C	85/107 (79%)	74 (87%)	11 (13%)	4	18
1	D	85/107 (79%)	76 (89%)	9 (11%)	6	26
1	E	87/107 (81%)	73 (84%)	14 (16%)	2	10
1	F	89/107 (83%)	79 (89%)	10 (11%)	6	24
1	G	89/107 (83%)	73 (82%)	16 (18%)	1	7
1	H	86/107 (80%)	72 (84%)	14 (16%)	2	10
1	I	91/107 (85%)	78 (86%)	13 (14%)	3	14
All	All	785/963 (82%)	677 (86%)	108 (14%)	3	16

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	73	LEU

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Mol	Chain	Res	Type
1	A	80	ASP
1	A	97	SER
1	A	158	GLU
1	B	58	CYS
1	B	61	LEU
1	B	71	LEU
1	B	80	ASP
1	B	83	GLU
1	B	88	LEU
1	B	96	HIS
1	B	97	SER
1	B	110	SER
1	B	111	ARG
1	B	112	VAL
1	B	135	LYS
1	B	154	LYS
1	B	156	LEU
1	B	158	GLU
1	B	159	GLU
1	C	58	CYS
1	C	71	LEU
1	C	80	ASP
1	C	88	LEU
1	C	91	ARG
1	C	92	GLN
1	C	96	HIS
1	C	109	LEU
1	C	133	VAL
1	C	150	ARG
1	C	156	LEU
1	D	71	LEU
1	D	88	LEU
1	D	110	SER
1	D	112	VAL
1	D	113	LEU
1	D	132	THR
1	D	138	SER
1	D	148	GLU
1	D	164	LEU
1	E	65	LYS
1	E	69	GLU
1	E	71	LEU

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Mol	Chain	Res	Type
1	E	76	MET
1	E	96	HIS
1	E	97	SER
1	E	112	VAL
1	E	113	LEU
1	E	118	SER
1	E	128	ASN
1	E	153	LYS
1	E	154	LYS
1	E	156	LEU
1	E	159	GLU
1	F	65	LYS
1	F	71	LEU
1	F	80	ASP
1	F	97	SER
1	F	110	SER
1	F	115	ARG
1	F	119	ARG
1	F	151	ILE
1	F	156	LEU
1	F	163	ASN
1	G	61	LEU
1	G	65	LYS
1	G	78	THR
1	G	88	LEU
1	G	91	ARG
1	G	96	HIS
1	G	98	LEU
1	G	111	ARG
1	G	113	LEU
1	G	123	LEU
1	G	128	ASN
1	G	129	GLU
1	G	131	CYS
1	G	138	SER
1	G	151	ILE
1	G	156	LEU
1	H	58	CYS
1	H	76	MET
1	H	83	GLU
1	H	85	VAL
1	H	88	LEU

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Mol	Chain	Res	Type
1	H	91	ARG
1	H	97	SER
1	H	109	LEU
1	H	111	ARG
1	H	112	VAL
1	H	128	ASN
1	H	146	ASP
1	H	151	ILE
1	H	164	LEU
1	I	62	GLU
1	I	64	GLU
1	I	71	LEU
1	I	76	MET
1	I	85	VAL
1	I	88	LEU
1	I	91	ARG
1	I	92	GLN
1	I	96	HIS
1	I	102	SER
1	I	112	VAL
1	I	150	ARG
1	I	155	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	81	HIS
1	E	96	HIS
1	H	128	ASN

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 (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(Å^2)	Q<0.9
1	A	105/119 (88%)	0.22	3 (2%)	51	28	35, 65, 104, 135	0
1	B	105/119 (88%)	0.15	1 (0%)	82	67	30, 58, 110, 157	0
1	C	106/119 (89%)	0.05	1 (0%)	84	69	43, 78, 102, 141	0
1	D	108/119 (90%)	0.33	3 (2%)	53	30	54, 78, 122, 161	0
1	E	108/119 (90%)	0.20	0	100	100	30, 73, 117, 145	0
1	F	104/119 (87%)	0.12	2 (1%)	66	46	46, 68, 109, 145	0
1	G	105/119 (88%)	0.21	3 (2%)	51	28	42, 71, 110, 125	0
1	H	103/119 (86%)	0.18	0	100	100	41, 62, 103, 123	0
1	I	103/119 (86%)	0.23	2 (1%)	66	46	51, 78, 110, 142	0
All	All	947/1071 (88%)	0.19	15 (1%)	72	51	30, 71, 112, 161	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	LEU	3.4
1	D	144	ASN	3.2
1	C	109	LEU	2.7
1	G	119	ARG	2.6
1	F	147	PRO	2.5
1	G	116	ALA	2.4
1	A	91	ARG	2.3
1	I	91	ARG	2.2
1	G	123	LEU	2.1
1	A	100	LEU	2.1
1	D	105	PHE	2.0
1	I	84	VAL	2.0
1	A	88	LEU	2.0
1	F	156	LEU	2.0
1	B	163	ASN	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 monosaccharides 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.