Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:26 PM GMT

PDB ID	:	1K78
Title	:	Pax5(1-149)+Ets-1(331-440)+DNA
Authors	:	Garvie, C.W.; Hagman, J.; Wolberger, C.
Deposited on	:	2001-10-18
Resolution	:	2.25 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 (i) symbol.

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

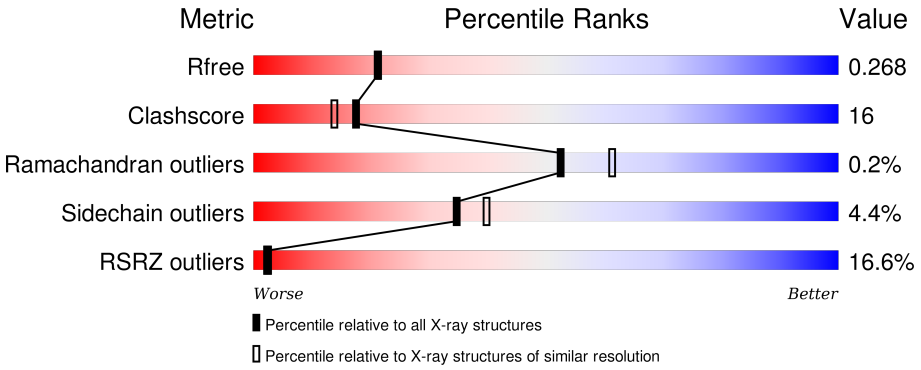
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	27	7%, 56%, 44%
1	G	27	19%, 41%, 59%
2	D	27	85%, 15%
2	H	27	33%, 33%, 67%
3	A	149	9%, 64%, 17%, 17%

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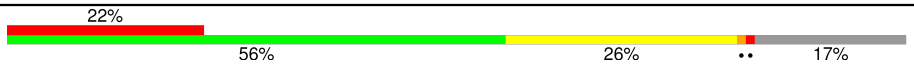
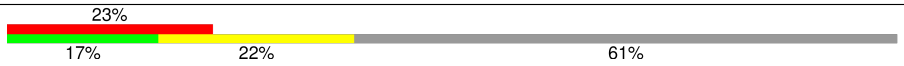
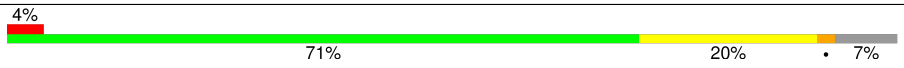
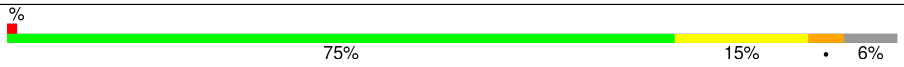
Mol	Chain	Length	Quality of chain
3	E	149	
3	I	149	
4	B	110	
4	F	110	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6901 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 DNA chain called Pax5/Ets Binding Site on the mb-1 promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	27	Total	C	N	O	P	0	0	0
			555	263	103	163	26			
1	G	27	Total	C	N	O	P	0	0	0
			555	263	103	163	26			

- Molecule 2 is a DNA chain called Pax5/Ets Binding Site on the mb-1 promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	27	Total	C	N	O	P	0	0	0
			546	259	104	157	26			
2	H	27	Total	C	N	O	P	0	0	0
			546	259	104	157	26			

- Molecule 3 is a protein called Paired Box Protein Pax5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	124	Total	C	N	O	S	0	2	0
			982	615	192	171	4			
3	E	124	Total	C	N	O	S	0	0	0
			968	606	186	172	4			
3	I	58	Total	C	N	O	S	0	0	0
			461	288	86	85	2			

- Molecule 4 is a protein called C-ets-1 Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	102	Total	C	N	O	S	0	4	0
			902	584	155	159	4			
4	F	103	Total	C	N	O	S	0	4	0
			902	583	157	158	4			

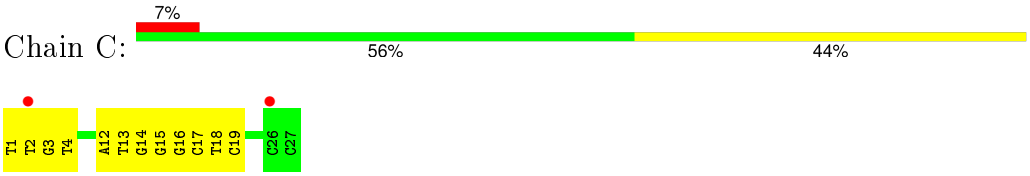
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	86	Total O 86 86	0	0
5	B	96	Total O 96 96	0	0
5	C	62	Total O 62 62	0	0
5	D	54	Total O 54 54	0	0
5	E	45	Total O 45 45	0	0
5	F	53	Total O 53 53	0	0
5	G	55	Total O 55 55	0	0
5	H	28	Total O 28 28	0	0
5	I	5	Total O 5 5	0	0

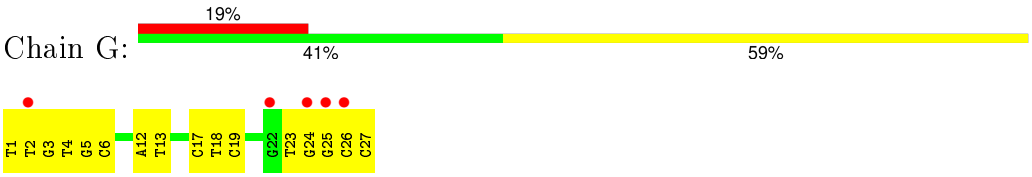
3 Residue-property plots (i)

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

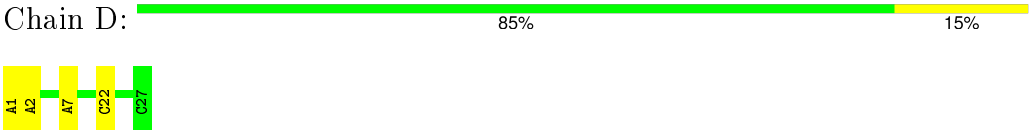
- Molecule 1: Pax5/Ets Binding Site on the mb-1 promoter



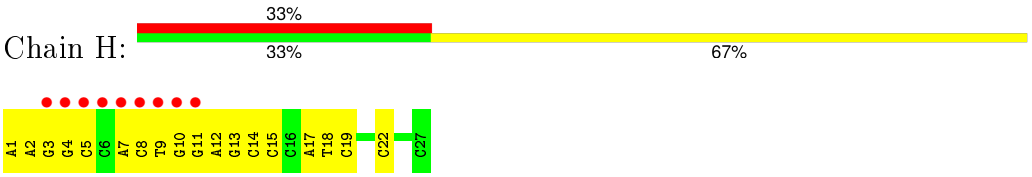
- Molecule 1: Pax5/Ets Binding Site on the mb-1 promoter



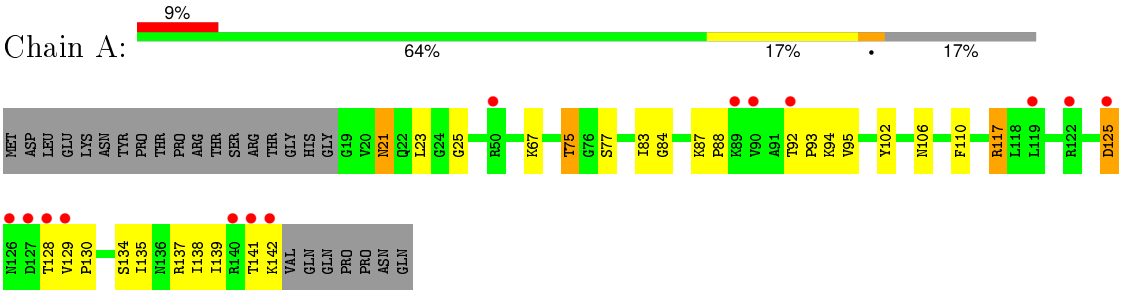
- Molecule 2: Pax5/Ets Binding Site on the mb-1 promoter



- Molecule 2: Pax5/Ets Binding Site on the mb-1 promoter

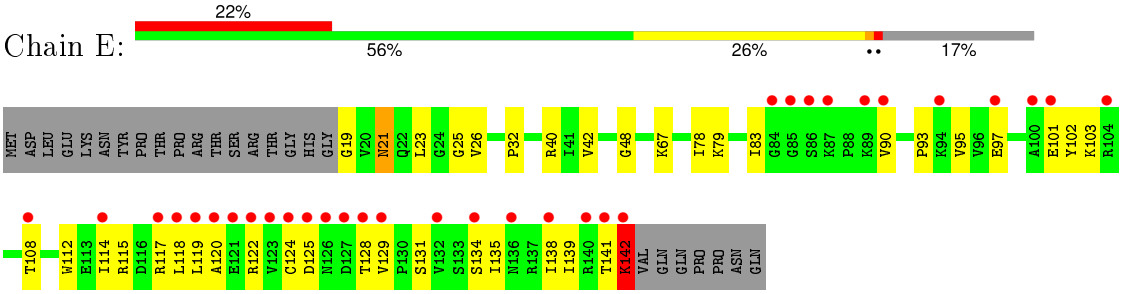


- Molecule 3: Paired Box Protein Pax5



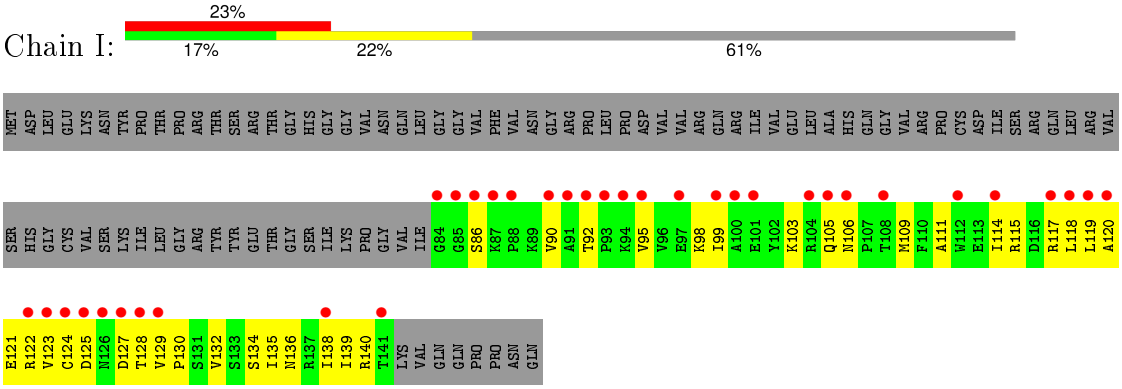
• Molecule 3: Paired Box Protein Pax5

Chain E:



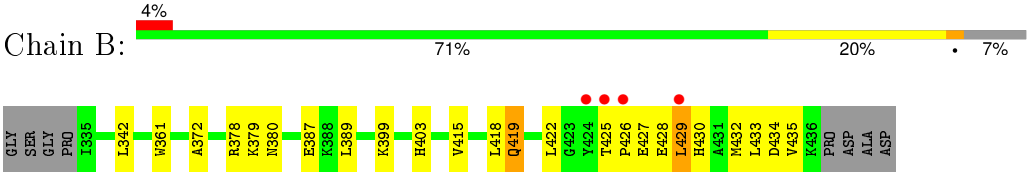
• Molecule 3: Paired Box Protein Pax5

Chain I:



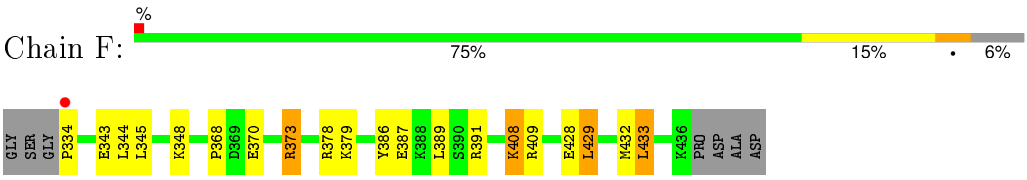
• Molecule 4: C-ets-1 Protein

Chain B:



• Molecule 4: C-ets-1 Protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.84Å 89.75Å 170.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.94 – 2.25 45.94 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.94-2.25) 98.7 (45.94-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.98 (at 2.24Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.260 0.237 , 0.268	Depositor DCC
R_{free} test set	2877 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 70.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 56835 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6901	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.41 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8511e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	C	0.37	0/622	0.74	0/960
1	G	0.35	0/622	0.69	0/960
2	D	0.39	0/612	0.75	0/941
2	H	0.37	0/612	0.77	0/941
3	A	0.38	0/1000	0.59	0/1350
3	E	0.36	0/984	0.62	1/1329 (0.1%)
3	I	0.28	0/468	0.49	0/632
4	B	0.41	0/926	0.61	0/1247
4	F	0.41	0/925	0.62	1/1246 (0.1%)
All	All	0.38	0/6771	0.66	2/9606 (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	1
2	D	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	142	LYS	N-CA-C	-7.68	90.26	111.00
4	F	334	PRO	N-CA-CB	5.33	109.70	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	14	DG	Sidechain
2	D	22	DC	Sidechain
2	H	22	DC	Sidechain

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	C	555	0	305	14	0
1	G	555	0	305	24	0
2	D	546	0	302	4	0
2	H	546	0	302	24	0
3	A	982	0	1032	30	0
3	E	968	0	1011	43	0
3	I	461	0	479	31	0
4	B	902	0	888	19	0
4	F	902	0	891	12	0
5	A	86	0	0	2	1
5	B	96	0	0	3	1
5	C	62	0	0	0	0
5	D	54	0	0	0	0
5	E	45	0	0	3	0
5	F	53	0	0	1	0
5	G	55	0	0	0	0
5	H	28	0	0	2	0
5	I	5	0	0	0	0
All	All	6901	0	5515	191	1

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 16.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:DA:H2"	2:H:8:DC:H5"	1.26	1.10
3:E:138:ILE:O	3:E:142:LYS:HB3	1.58	1.03
2:H:8:DC:H2"	2:H:9:DT:H5'	1.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:DT:H2"	2:H:19:DC:H5'	1.45	0.97
3:A:75:THR:HG22	3:A:77:SER:H	1.38	0.89
2:H:7:DA:C2'	2:H:8:DC:H5"	2.05	0.84
3:I:90:VAL:HG22	3:I:130:PRO:HG3	1.61	0.82
3:I:119:LEU:HD13	3:I:129:VAL:HG21	1.62	0.81
3:I:105:GLN:NE2	3:I:117:ARG:HH22	1.79	0.80
3:A:21:ASN:ND2	3:A:25:GLY:H	1.82	0.77
4:B:427:GLU:CD	4:B:427:GLU:H	1.89	0.76
3:A:106:ASN:ND2	4:F:408:LYS:HE3	2.01	0.75
3:I:125:ASP:O	3:I:129:VAL:HG23	1.86	0.75
2:H:8:DC:H2"	2:H:9:DT:C5'	2.17	0.74
4:B:387[B]:GLU:HG3	5:B:472:HOH:O	1.87	0.74
4:B:425:THR:OG1	4:B:428:GLU:HB2	1.86	0.74
3:A:21:ASN:HD21	3:A:25:GLY:H	1.36	0.72
2:H:17:DA:H2"	2:H:18:DT:H5"	1.73	0.71
1:G:3:DG:H2'	1:G:4:DT:H72	1.72	0.71
3:I:95:VAL:HG13	3:I:118:LEU:HD21	1.73	0.70
4:B:387[A]:GLU:HG3	5:B:472:HOH:O	1.90	0.70
3:E:142:LYS:C	3:E:142:LYS:HD2	2.10	0.70
2:H:11:DG:H2"	2:H:12:DA:C8	2.26	0.69
2:H:11:DG:H2"	2:H:12:DA:H8	1.57	0.69
3:A:135:ILE:O	3:A:139:ILE:HG12	1.95	0.67
2:H:4:DG:H2"	2:H:5:DC:C5'	2.25	0.67
3:E:21:ASN:HD22	3:E:23:LEU:H	1.42	0.67
1:G:18:DT:H2"	1:G:19:DC:C5'	2.25	0.66
3:I:134:SER:O	3:I:138:ILE:HG12	1.95	0.66
1:C:18:DT:H2"	1:C:19:DC:H5'	1.79	0.65
3:A:75:THR:HG22	3:A:77:SER:N	2.11	0.65
3:I:90:VAL:HG21	3:I:130:PRO:HA	1.78	0.65
3:E:21:ASN:ND2	3:E:23:LEU:H	1.95	0.64
4:F:386:TYR:HE1	5:F:469:HOH:O	1.80	0.64
3:A:21:ASN:HD22	3:A:21:ASN:C	2.00	0.64
3:E:93:PRO:O	3:E:97:GLU:HG3	1.99	0.63
1:C:17:DC:H2'	1:C:18:DT:H71	1.80	0.63
4:B:378[A]:ARG:NH1	5:B:504:HOH:O	2.31	0.63
3:E:119:LEU:HG	3:E:129:VAL:HG21	1.81	0.62
3:A:23:LEU:HD21	4:B:399:LYS:HE3	1.81	0.62
3:E:125:ASP:H	3:E:128:THR:HB	1.63	0.62
1:G:12:DA:H2"	1:G:13:DT:H5'	1.82	0.61
4:B:430:HIS:HB3	4:B:435:VAL:HB	1.81	0.61
2:H:4:DG:H2"	2:H:5:DC:H5'	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:102:TYR:CZ	3:A:117:ARG:HD2	2.34	0.61
3:A:125:ASP:H	3:A:128:THR:HB	1.66	0.61
3:E:32:PRO:HG3	3:E:83:ILE:HD11	1.82	0.61
4:B:425:THR:OG1	4:B:428:GLU:CB	2.49	0.61
1:C:15:DG:H2"	1:C:16:DG:C8	2.37	0.60
4:F:343:GLU:OE2	4:F:378[B]:ARG:NH2	2.35	0.59
4:F:429[B]:LEU:HD13	4:F:433:LEU:HD22	1.85	0.59
1:C:18:DT:H2"	1:C:19:DC:C5'	2.33	0.58
1:C:3:DG:H2'	1:C:4:DT:H72	1.84	0.58
3:I:90:VAL:HG23	3:I:128:THR:O	2.03	0.58
3:E:21:ASN:C	3:E:21:ASN:HD22	2.06	0.58
2:H:19:DC:OP1	4:F:379:LYS:HE2	2.04	0.57
1:G:18:DT:H2"	1:G:19:DC:H5'	1.86	0.56
2:H:3:DG:H2"	2:H:4:DG:C8	2.40	0.56
3:A:137:ARG:NH1	5:A:206:HOH:O	2.38	0.56
4:F:370:GLU:OE2	4:F:373:ARG:NH1	2.39	0.56
3:E:103:LYS:HE3	3:E:139:ILE:HD13	1.87	0.56
2:H:8:DC:H2'	2:H:9:DT:H71	1.87	0.56
3:E:141:THR:HG22	3:E:141:THR:O	2.06	0.55
3:E:114:ILE:O	3:E:118:LEU:HB2	2.07	0.55
1:G:1:DT:H2"	1:G:2:DT:H5"	1.89	0.55
3:E:79:LYS:HG2	5:E:169:HOH:O	2.06	0.55
2:H:18:DT:H5'	5:H:90:HOH:O	2.07	0.55
1:G:5:DG:H2"	1:G:6:DC:H5'	1.89	0.54
3:E:21:ASN:HD21	3:E:25:GLY:H	1.55	0.54
2:H:1:DA:H2"	2:H:2:DA:C8	2.42	0.54
3:A:21:ASN:ND2	3:A:23:LEU:H	2.06	0.54
1:G:26:DC:H2"	1:G:27:DC:C6	2.43	0.54
3:E:120:ALA:C	3:E:122:ARG:H	2.12	0.54
4:B:425:THR:HG1	4:B:428:GLU:HB2	1.73	0.53
1:G:17:DC:H2'	1:G:18:DT:H72	1.90	0.53
3:E:124:CYS:HB2	3:E:129:VAL:CG2	2.39	0.53
3:A:138:ILE:O	3:A:142:LYS:O	2.26	0.53
2:H:9:DT:H2"	2:H:10:DG:C8	2.43	0.53
3:A:75:THR:CG2	3:A:77:SER:HB3	2.39	0.53
1:G:18:DT:H2"	1:G:19:DC:H5"	1.90	0.53
3:I:121:GLU:HB2	3:I:123:VAL:HG23	1.91	0.53
3:E:112:TRP:HB2	3:E:115:ARG:HH21	1.73	0.53
2:H:10:DG:H2"	2:H:11:DG:C8	2.44	0.52
1:C:18:DT:H1'	1:C:19:DC:H5"	1.90	0.52
3:A:92:THR:HG23	3:A:93:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:111:ALA:CB	3:I:132:VAL:HG13	2.39	0.52
3:I:120:ALA:C	3:I:122:ARG:H	2.13	0.52
1:G:24:DG:H2"	1:G:25:DG:C5'	2.40	0.52
1:C:12:DA:H1'	1:C:13:DT:H5"	1.92	0.52
1:C:17:DC:C2'	1:C:18:DT:H71	2.40	0.51
3:E:124:CYS:HB2	3:E:129:VAL:HG22	1.92	0.51
2:D:1:DA:H2"	2:D:2:DA:C8	2.46	0.51
4:B:372:ALA:HA	4:B:389[B]:LEU:HD12	1.93	0.51
1:C:17:DC:H2"	1:C:18:DT:C6	2.46	0.50
3:I:114:ILE:O	3:I:118:LEU:HB2	2.11	0.50
3:E:21:ASN:ND2	3:E:25:GLY:H	2.08	0.50
2:D:1:DA:H4'	3:A:110:PHE:CE1	2.47	0.50
3:E:115:ARG:HG3	3:E:129:VAL:HG11	1.93	0.50
1:G:18:DT:C2'	1:G:19:DC:H5"	2.41	0.50
3:A:92:THR:HG22	3:A:94:LYS:H	1.76	0.50
3:I:95:VAL:O	3:I:99:ILE:HG13	2.12	0.50
3:E:78:ILE:C	3:E:78:ILE:HD12	2.33	0.49
2:H:3:DG:H2"	2:H:4:DG:H8	1.77	0.49
3:E:102:TYR:CZ	3:E:117:ARG:HD2	2.47	0.49
3:A:94:LYS:HG3	3:A:95:VAL:N	2.28	0.49
4:B:403:HIS:CD2	4:B:415:VAL:HG11	2.47	0.49
5:H:91:HOH:O	4:F:391:ARG:HG3	2.13	0.49
4:B:429:LEU:O	4:B:433:LEU:HG	2.13	0.49
4:F:389[A]:LEU:O	4:F:389[A]:LEU:HD23	2.13	0.49
3:E:102:TYR:HD1	3:E:114:ILE:HG23	1.77	0.48
3:I:90:VAL:HG21	3:I:130:PRO:CA	2.43	0.48
2:H:14:DC:H2"	2:H:15:DC:C6	2.48	0.48
1:G:5:DG:H2"	1:G:6:DC:C5'	2.43	0.48
3:I:128:THR:O	3:I:128:THR:HG22	2.14	0.48
1:G:5:DG:H4'	3:A:110:PHE:CZ	2.48	0.48
4:B:428:GLU:O	4:B:432:MET:HG3	2.14	0.48
2:D:7:DA:N3	3:I:86:SER:HB3	2.29	0.48
3:E:138:ILE:O	3:E:142:LYS:CB	2.47	0.47
3:E:97:GLU:O	3:E:101:GLU:HG3	2.13	0.47
3:A:87:LYS:HE2	3:A:88:PRO:HD3	1.95	0.47
3:I:92:THR:OG1	3:I:95:VAL:HG23	2.14	0.47
1:C:12:DA:H2"	1:C:13:DT:C5'	2.44	0.47
3:I:135:ILE:O	3:I:139:ILE:HG13	2.15	0.47
2:H:4:DG:H2"	2:H:5:DC:H5"	1.93	0.47
1:G:24:DG:H2"	1:G:25:DG:H5'	1.96	0.47
1:G:18:DT:H1'	1:G:19:DC:H5"	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:342:LEU:HD21	4:B:422:LEU:HD21	1.96	0.47
3:A:67[A]:LYS:NZ	5:A:188:HOH:O	2.47	0.47
3:E:95:VAL:HG22	3:E:124:CYS:SG	2.55	0.46
3:I:103:LYS:HE3	3:I:139:ILE:HD13	1.98	0.46
3:E:119:LEU:CG	3:E:129:VAL:HG21	2.44	0.46
1:C:3:DG:C2'	1:C:4:DT:H72	2.45	0.46
3:I:136:ASN:O	3:I:140:ARG:HG3	2.15	0.46
3:E:124:CYS:HB3	3:E:128:THR:HB	1.98	0.46
4:B:361:TRP:CE2	4:B:426:PRO:HG3	2.51	0.46
1:C:12:DA:H2"	1:C:13:DT:H5'	1.96	0.46
3:I:95:VAL:CG1	3:I:118:LEU:HD21	2.43	0.46
3:E:135:ILE:O	3:E:139:ILE:HG13	2.15	0.46
3:E:119:LEU:CD2	3:E:129:VAL:HG21	2.45	0.45
3:E:134:SER:O	3:E:138:ILE:HG13	2.17	0.45
4:B:379:LYS:O	4:B:380:ASN:HB3	2.16	0.45
4:B:419:GLN:HB3	4:B:419:GLN:HE21	1.50	0.45
3:I:125:ASP:C	3:I:127:ASP:H	2.20	0.45
1:C:19:DC:H6	1:C:19:DC:H5'	1.81	0.45
3:E:19:GLY:O	3:E:26:VAL:HA	2.18	0.44
1:G:17:DC:H2"	1:G:18:DT:C6	2.52	0.44
3:I:124:CYS:HB2	3:I:129:VAL:HG22	1.99	0.44
3:E:21:ASN:HD22	3:E:23:LEU:N	2.12	0.44
3:E:120:ALA:C	3:E:122:ARG:N	2.69	0.44
3:I:125:ASP:C	3:I:127:ASP:N	2.71	0.44
3:E:40:ARG:HG2	5:E:176:HOH:O	2.18	0.44
3:E:142:LYS:CD	3:E:142:LYS:C	2.81	0.43
3:A:129:VAL:HA	3:A:130:PRO:HD3	1.89	0.43
4:F:368:PRO:HB2	4:F:386:TYR:CD1	2.53	0.43
4:F:348:LYS:HE2	4:F:433:LEU:HA	2.01	0.43
2:H:12:DA:H2"	2:H:13:DG:C8	2.53	0.43
3:E:48:GLY:HA2	5:E:175:HOH:O	2.18	0.43
1:G:23:DT:OP1	3:E:90:VAL:HG22	2.19	0.43
3:A:83:ILE:HG22	3:A:84:GLY:N	2.34	0.43
3:A:21:ASN:C	3:A:21:ASN:ND2	2.72	0.43
1:G:19:DC:H6	1:G:19:DC:H5'	1.83	0.43
3:I:115:ARG:HG2	3:I:129:VAL:CG1	2.49	0.42
1:G:26:DC:H2'	1:G:27:DC:C5	2.54	0.42
4:F:389[A]:LEU:C	4:F:389[A]:LEU:HD23	2.40	0.42
3:A:134:SER:O	3:A:138:ILE:HG13	2.18	0.42
3:I:111:ALA:HB1	3:I:132:VAL:HG13	2.01	0.42
3:A:75:THR:HG21	3:A:77:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:DA:H1'	1:G:13:DT:H5"	2.00	0.42
2:H:4:DG:C2'	2:H:5:DC:H5"	2.49	0.42
3:E:122:ARG:HD2	3:E:122:ARG:HA	1.82	0.42
3:E:131:SER:O	3:E:135:ILE:HG13	2.20	0.42
3:I:111:ALA:HB3	3:I:132:VAL:HG13	2.00	0.42
3:I:106:ASN:O	3:I:109:MET:HG3	2.20	0.42
4:F:428:GLU:O	4:F:432:MET:HE3	2.20	0.42
1:C:1:DT:H2"	1:C:2:DT:H5'	2.02	0.42
3:I:125:ASP:H	3:I:128:THR:HB	1.85	0.41
1:G:17:DC:C2'	1:G:18:DT:H72	2.50	0.41
4:B:425:THR:O	4:B:428:GLU:HB3	2.21	0.41
3:E:115:ARG:HG3	3:E:129:VAL:CG1	2.50	0.41
3:E:42:VAL:HG21	3:E:78:ILE:HG22	2.02	0.41
1:G:3:DG:C2'	1:G:4:DT:H72	2.47	0.41
3:A:137:ARG:HH11	3:A:137:ARG:HG2	1.85	0.41
2:H:14:DC:O3'	3:E:32:PRO:HA	2.21	0.41
2:D:1:DA:H4'	3:A:110:PHE:CD1	2.56	0.41
3:A:23:LEU:CD2	4:B:399:LYS:HE3	2.47	0.40
3:I:98:LYS:HD3	3:I:98:LYS:HA	1.93	0.40
2:H:7:DA:C3'	2:H:8:DC:H5"	2.45	0.40
3:I:95:VAL:HG22	3:I:124:CYS:SG	2.61	0.40
3:A:87:LYS:HA	3:A:87:LYS:HE2	2.03	0.40
1:G:3:DG:H2'	1:G:4:DT:C7	2.49	0.40
1:G:26:DC:C2'	1:G:27:DC:C6	3.05	0.40

All (1) 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)
5:A:150:HOH:O	5:B:460:HOH:O[4_555]	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
3	A	124/149 (83%)	122 (98%)	1 (1%)	1 (1%)	24 21
3	E	122/149 (82%)	118 (97%)	4 (3%)	0	100 100
3	I	56/149 (38%)	51 (91%)	5 (9%)	0	100 100
4	B	104/110 (94%)	102 (98%)	2 (2%)	0	100 100
4	F	105/110 (96%)	103 (98%)	2 (2%)	0	100 100
All	All	511/667 (77%)	496 (97%)	14 (3%)	1 (0%)	52 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	THR

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
3	A	109/131 (83%)	105 (96%)	4 (4%)	41 50
3	E	108/131 (82%)	104 (96%)	4 (4%)	41 50
3	I	52/131 (40%)	52 (100%)	0	100 100
4	B	96/98 (98%)	92 (96%)	4 (4%)	36 42
4	F	96/98 (98%)	87 (91%)	9 (9%)	11 8
All	All	461/589 (78%)	440 (95%)	21 (5%)	35 37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	21	ASN
3	A	75	THR
3	A	117	ARG
3	A	125	ASP
4	B	418	LEU

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Mol	Chain	Res	Type
4	B	419	GLN
4	B	429	LEU
4	B	434	ASP
3	E	21	ASN
3	E	67	LYS
3	E	108	THR
3	E	142	LYS
4	F	344	LEU
4	F	345	LEU
4	F	373	ARG
4	F	387	GLU
4	F	408	LYS
4	F	409	ARG
4	F	429[A]	LEU
4	F	429[B]	LEU
4	F	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	21	ASN
3	A	39	GLN
3	A	106	ASN
4	B	380	ASN
4	B	403	HIS
4	B	419	GLN
3	E	21	ASN
3	E	46	HIS
4	F	380	ASN
3	I	105	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

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	C	27/27 (100%)	0.77	2 (7%) 17 18	21, 42, 75, 127	0
1	G	27/27 (100%)	1.08	5 (18%) 2 1	23, 46, 87, 110	0
2	D	27/27 (100%)	0.52	0 100 100	19, 41, 65, 68	0
2	H	27/27 (100%)	1.44	9 (33%) 0 0	22, 46, 95, 99	0
3	A	124/149 (83%)	0.75	14 (11%) 7 7	15, 39, 76, 99	0
3	E	124/149 (83%)	1.51	33 (26%) 1 1	18, 51, 107, 114	0
3	I	58/149 (38%)	2.83	35 (60%) 0 0	51, 84, 106, 114	0
4	B	102/110 (92%)	0.78	4 (3%) 43 47	16, 34, 72, 94	0
4	F	103/110 (93%)	0.61	1 (0%) 84 85	15, 28, 46, 67	0
All	All	619/775 (79%)	1.11	103 (16%) 2 2	15, 41, 98, 127	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	128	THR	8.0
3	I	141	THR	7.3
3	I	125	ASP	6.8
3	I	129	VAL	6.4
3	I	122	ARG	6.2
3	I	123	VAL	6.1
3	I	101	GLU	5.9
3	E	126	ASN	5.8
3	E	127	ASP	5.8
3	E	129	VAL	5.7
3	E	123	VAL	5.7
3	I	104	ARG	5.5
3	E	120	ALA	5.4
3	I	97	GLU	5.3
3	E	141	THR	5.2

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Mol	Chain	Res	Type	RSRZ
3	E	89	LYS	5.1
3	I	99	ILE	5.0
3	I	94	LYS	5.0
3	E	118	LEU	4.9
1	C	2	DT	4.9
3	E	125	ASP	4.8
3	A	142	LYS	4.8
3	I	119	LEU	4.8
3	E	122	ARG	4.7
2	H	5	DC	4.6
3	I	91	ALA	4.6
3	E	104	ARG	4.5
3	I	87	LYS	4.5
3	I	124	CYS	4.4
3	I	90	VAL	4.4
2	H	6	DC	4.3
2	H	8	DC	4.3
3	E	97	GLU	4.2
3	I	127	ASP	4.2
3	A	125	ASP	4.1
3	E	94	LYS	3.8
3	I	92	THR	3.8
3	I	106	ASN	3.7
3	A	128	THR	3.7
3	I	120	ALA	3.7
3	I	105	GLN	3.6
2	H	11	DG	3.6
3	I	128	THR	3.6
3	I	85	GLY	3.5
3	E	114	ILE	3.5
3	I	93	PRO	3.4
3	I	138	ILE	3.4
3	E	124	CYS	3.4
3	E	142	LYS	3.3
3	I	84	GLY	3.3
3	E	86	SER	3.3
3	E	140	ARG	3.2
1	G	25	DG	3.1
2	H	10	DG	3.1
3	A	127	ASP	3.0
3	E	85	GLY	3.0
3	E	134	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	7	DA	3.0
3	E	121	GLU	3.0
3	E	138	ILE	2.9
2	H	4	DG	2.9
3	E	119	LEU	2.9
2	H	3	DG	2.8
3	I	126	ASN	2.8
1	G	2	DT	2.6
4	B	424	TYR	2.6
4	B	429	LEU	2.6
3	A	50[A]	ARG	2.6
3	I	95	VAL	2.6
4	F	334	PRO	2.5
3	I	118	LEU	2.5
3	A	140	ARG	2.5
3	A	141	THR	2.5
2	H	9	DT	2.5
1	C	26	DC	2.4
3	A	92	THR	2.4
3	I	100	ALA	2.4
3	I	88	PRO	2.4
3	A	129	VAL	2.4
3	E	87	LYS	2.4
3	I	112	TRP	2.4
3	E	136	ASN	2.3
3	I	86	SER	2.3
3	E	90	VAL	2.3
3	A	89	LYS	2.3
3	E	100	ALA	2.2
3	E	132	VAL	2.1
1	G	26	DC	2.1
1	G	22	DG	2.1
3	A	122	ARG	2.1
3	E	108	THR	2.1
1	G	24	DG	2.1
3	I	117	ARG	2.1
3	E	101	GLU	2.1
3	E	84	GLY	2.1
3	E	117	ARG	2.1
3	I	114	ILE	2.1
4	B	426	PRO	2.0
3	A	90	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	108	THR	2.0
3	A	126	ASN	2.0
4	B	425	THR	2.0
3	A	119	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.