Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2016 – 12:52 PM EST

PDB ID	:	5T1J
Title	:	Crystal Structure of the Tbox DNA binding domain of the transcription factor T-bet
Authors	:	Liu, C.F.; Brandt, G.S.; Hoang, Q.; Hwang, E.S.; Naumova, N.; Lazarevic, V.; Dekker, J.; Glimcher, L.H.; Ringe, D.; Petsko, G.A.
Deposited on	:	2016-08-19
Resolution	:	2.95 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:

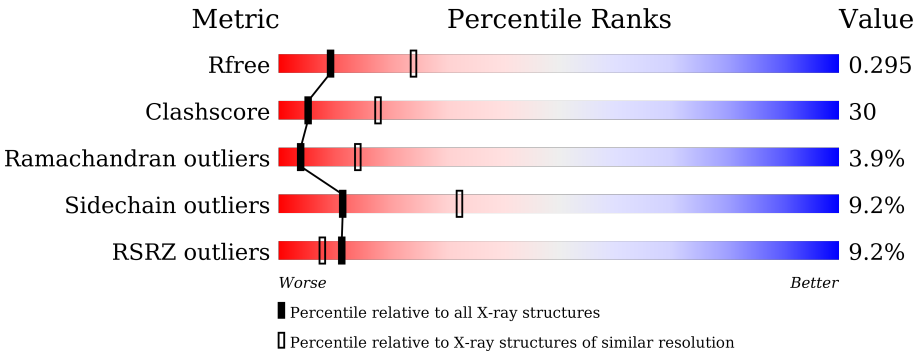
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.95 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	A	204	10% 43% 43% 8% 6%
1	B	204	10% 37% 49% 8% 6%
2	C	24	46% 46% 8%
2	D	24	42% 54% .
2	E	24	4% 46% 38% 17%
2	F	24	4% 25% 67% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5062 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 T-box transcription factor TBX21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1553	983	282	280	8			
1	B	192	Total	C	N	O	S	0	0	0
			1553	983	282	280	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9JKD8
A	125	ARG	-	expression tag	UNP Q9JKD8
A	126	GLY	-	expression tag	UNP Q9JKD8
A	127	SER	-	expression tag	UNP Q9JKD8
A	128	HIS	-	expression tag	UNP Q9JKD8
A	129	HIS	-	expression tag	UNP Q9JKD8
A	130	HIS	-	expression tag	UNP Q9JKD8
A	131	HIS	-	expression tag	UNP Q9JKD8
A	132	HIS	-	expression tag	UNP Q9JKD8
A	133	HIS	-	expression tag	UNP Q9JKD8
A	134	GLY	-	expression tag	UNP Q9JKD8
A	135	SER	-	expression tag	UNP Q9JKD8
B	124	MET	-	initiating methionine	UNP Q9JKD8
B	125	ARG	-	expression tag	UNP Q9JKD8
B	126	GLY	-	expression tag	UNP Q9JKD8
B	127	SER	-	expression tag	UNP Q9JKD8
B	128	HIS	-	expression tag	UNP Q9JKD8
B	129	HIS	-	expression tag	UNP Q9JKD8
B	130	HIS	-	expression tag	UNP Q9JKD8
B	131	HIS	-	expression tag	UNP Q9JKD8
B	132	HIS	-	expression tag	UNP Q9JKD8
B	133	HIS	-	expression tag	UNP Q9JKD8
B	134	GLY	-	expression tag	UNP Q9JKD8
B	135	SER	-	expression tag	UNP Q9JKD8

- Molecule 2 is a DNA chain called DNA.

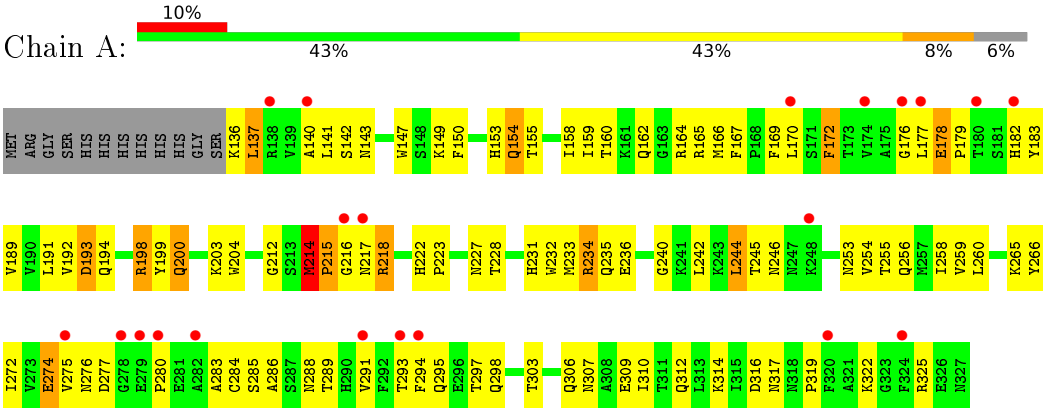
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	24	Total	C	N	O	P	0	0	0
			489	236	88	142	23			
2	D	24	Total	C	N	O	P	0	0	0
			489	236	88	142	23			
2	E	24	Total	C	N	O	P	0	0	0
			489	236	88	142	23			
2	F	24	Total	C	N	O	P	0	0	0
			489	236	88	142	23			

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.

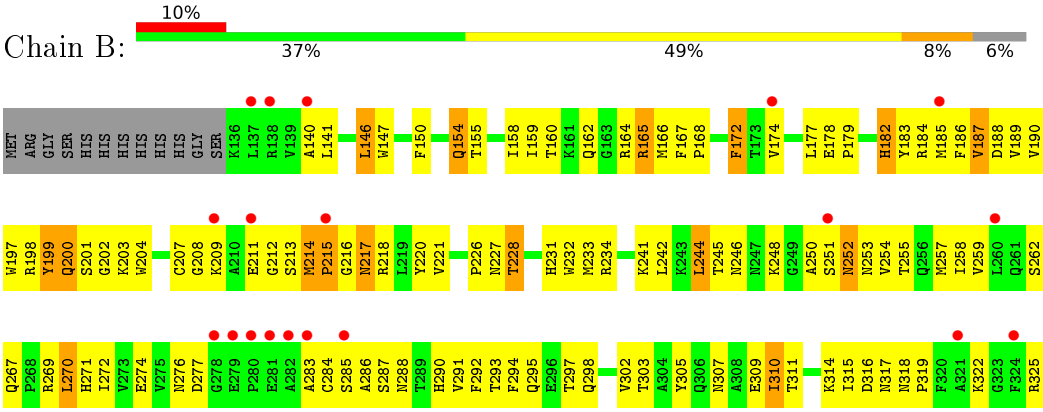
- Molecule 1: T-box transcription factor TBX21

Chain A:



- Molecule 1: T-box transcription factor TBX21

Chain B:



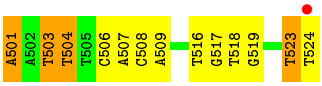
- Molecule 2: DNA

Chain C:

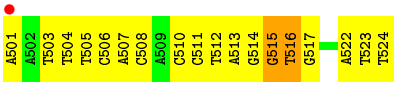
- Molecule 2: DNA

Chain D:

• Molecule 2: DNA



• Molecule 2: DNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	70.45Å 70.45Å 438.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.70 – 2.95 43.70 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.8 (43.70-2.95) 87.9 (43.70-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.266 , 0.294 0.266 , 0.295	Depositor DCC
R_{free} test set	1154 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	81.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5062	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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	0.63	0/1594	0.95	2/2157 (0.1%)
1	B	0.60	0/1594	0.88	0/2157
2	C	1.05	0/548	1.16	4/844 (0.5%)
2	D	1.03	0/548	1.19	2/844 (0.2%)
2	E	1.22	4/548 (0.7%)	1.18	4/844 (0.5%)
2	F	1.01	1/548 (0.2%)	1.20	2/844 (0.2%)
All	All	0.84	5/5380 (0.1%)	1.04	14/7690 (0.2%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	523	DT	C1'-N1	8.86	1.60	1.49
2	E	501	DA	N9-C4	6.30	1.41	1.37
2	F	522	DA	C3'-O3'	-5.86	1.36	1.44
2	E	504	DT	C1'-N1	5.41	1.56	1.49
2	E	523	DT	P-O5'	5.16	1.65	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	MET	C-N-CD	-13.72	90.42	120.60
2	E	523	DT	O4'-C1'-N1	8.42	113.89	108.00
1	A	214	MET	C-N-CA	8.00	155.61	122.00
2	D	517	DG	O5'-P-OP2	-6.03	100.28	105.70
2	C	523	DT	OP1-P-O3'	5.60	117.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	515	DG	O4'-C1'-N9	-5.53	104.13	108.00
2	C	523	DT	P-O3'-C3'	5.45	126.25	119.70
2	E	503	DT	C1'-O4'-C4'	-5.45	104.65	110.10
2	C	523	DT	O4'-C1'-C2'	-5.42	101.57	105.90
2	F	516	DT	N3-C4-O4	5.37	123.12	119.90
2	E	523	DT	C1'-O4'-C4'	-5.36	104.74	110.10
2	E	506	DC	O5'-P-OP2	-5.22	101.00	105.70
2	C	524	DT	O5'-P-OP2	-5.21	101.01	105.70
2	D	517	DG	OP2-P-O3'	5.11	116.44	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	GLN	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	1553	0	1512	114	0
1	B	1553	0	1512	122	0
2	C	489	0	274	11	0
2	D	489	0	274	15	0
2	E	489	0	274	11	0
2	F	489	0	274	17	0
All	All	5062	0	4120	267	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 30.

All (267) 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:B:188:ASP:HB2	1:B:217:ASN:HD21	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:HIS:HA	1:A:234:ARG:HG3	1.41	1.00
1:A:154:GLN:HG3	1:A:204:TRP:CD1	2.04	0.92
1:B:251:SER:C	1:B:252:ASN:HD22	1.75	0.90
1:B:218:ARG:HH21	1:B:259:VAL:HG11	1.39	0.87
1:B:315:ILE:O	1:B:325:ARG:NH2	2.08	0.86
1:A:200:GLN:N	1:A:200:GLN:HE21	1.73	0.84
1:B:154:GLN:HG3	1:B:204:TRP:CD1	2.13	0.84
1:A:136:LYS:HG2	1:A:137:LEU:HG	1.60	0.82
1:A:228:THR:HG23	1:A:231:HIS:H	1.45	0.82
1:B:316:ASP:OD1	1:B:317:ASN:ND2	2.13	0.82
1:B:188:ASP:HB2	1:B:217:ASN:ND2	1.96	0.81
1:A:316:ASP:OD1	1:A:317:ASN:ND2	2.17	0.78
1:A:158:ILE:HG23	1:A:164:ARG:HG2	1.66	0.77
1:A:218:ARG:HH11	1:A:218:ARG:HG2	1.50	0.76
1:A:187:VAL:HG23	1:A:270:LEU:HB2	1.66	0.76
1:A:166:MET:HG3	1:A:244:LEU:HD11	1.67	0.76
1:A:183:TYR:HD1	1:A:274:GLU:HB3	1.51	0.75
1:A:141:LEU:HB2	1:A:294:PHE:CE1	2.22	0.74
1:A:183:TYR:CD1	1:A:274:GLU:HB3	2.22	0.74
1:A:242:LEU:HD21	1:A:258:ILE:HG13	1.69	0.73
1:B:242:LEU:HD21	1:B:258:ILE:HG13	1.70	0.73
1:B:187:VAL:HG23	1:B:270:LEU:HB2	1.70	0.73
1:B:165:ARG:HE	2:D:515:DG:H5"	1.54	0.72
1:B:322:LYS:HB3	1:B:325:ARG:HH12	1.53	0.72
1:A:284:CYS:N	1:A:285:SER:HA	2.02	0.72
1:A:256:GLN:OE1	1:B:253:ASN:ND2	2.23	0.70
1:A:136:LYS:NZ	1:A:137:LEU:HD11	2.07	0.70
2:E:507:DA:H1'	2:E:508:DC:H5'	1.74	0.70
1:B:274:GLU:H	1:B:288:ASN:HD21	1.37	0.69
1:A:214:MET:HB3	1:A:216:GLY:N	2.07	0.69
1:B:141:LEU:HB2	1:B:294:PHE:CE1	2.26	0.69
1:B:192:VAL:HB	1:B:265:LYS:HG3	1.75	0.69
2:C:523:DT:H4'	2:C:524:DT:OP1	1.91	0.69
1:B:158:ILE:HG23	1:B:164:ARG:HG2	1.74	0.69
1:A:154:GLN:HG3	1:A:204:TRP:HD1	1.56	0.68
1:A:217:ASN:HB3	1:B:184:ARG:HH22	1.57	0.68
1:B:154:GLN:HG3	1:B:204:TRP:HD1	1.60	0.67
2:E:517:DG:H1	2:F:508:DC:H42	1.41	0.67
1:A:141:LEU:HB2	1:A:294:PHE:HE1	1.58	0.66
1:A:316:ASP:HA	1:A:322:LYS:HE3	1.78	0.66
1:B:319:PRO:HA	1:B:322:LYS:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:CZ	2:F:515:DG:H5"	2.26	0.65
1:A:307:ASN:OD1	1:A:309:GLU:HG2	1.97	0.65
1:A:166:MET:CG	1:A:244:LEU:HD11	2.28	0.64
1:B:252:ASN:N	1:B:252:ASN:HD22	1.95	0.64
1:B:198:ARG:HB2	1:B:207:CYS:SG	2.38	0.64
1:B:316:ASP:HA	1:B:325:ARG:HE	1.62	0.64
1:A:271:HIS:HD2	1:A:291:VAL:HG22	1.63	0.63
2:F:514:DG:H2"	2:F:515:DG:C8	2.34	0.63
2:C:507:DA:H1'	2:C:508:DC:H5'	1.81	0.62
2:E:516:DT:H2"	2:E:517:DG:C8	2.35	0.62
1:B:160:THR:HG22	1:B:162:GLN:H	1.64	0.62
1:B:200:GLN:O	1:B:203:LYS:N	2.32	0.62
1:A:276:ASN:ND2	1:A:286:ALA:HB3	2.15	0.62
2:F:507:DA:H1'	2:F:508:DC:H5'	1.82	0.61
2:C:516:DT:H2"	2:C:517:DG:C8	2.35	0.61
1:B:182:HIS:HB3	1:B:228:THR:HA	1.82	0.61
2:D:507:DA:H1'	2:D:508:DC:H5'	1.82	0.61
2:F:506:DC:H2"	2:F:507:DA:C8	2.35	0.61
1:B:303:THR:OG1	2:C:504:DT:OP2	2.11	0.61
2:D:506:DC:H2"	2:D:507:DA:C8	2.36	0.61
1:B:197:TRP:HZ2	1:B:265:LYS:HZ2	1.48	0.60
1:B:255:THR:HB	1:B:257:MET:HG2	1.83	0.60
1:B:316:ASP:HA	1:B:325:ARG:HH21	1.66	0.60
1:A:269:ARG:HG3	1:A:293:THR:HG22	1.84	0.59
1:B:253:ASN:OD1	1:B:254:VAL:N	2.34	0.59
1:B:183:TYR:CD1	1:B:274:GLU:HG2	2.37	0.59
1:B:316:ASP:OD1	1:B:317:ASN:N	2.35	0.59
1:A:217:ASN:HB3	1:B:184:ARG:NH2	2.18	0.58
1:B:283:ALA:O	1:B:285:SER:N	2.32	0.58
2:D:516:DT:H2"	2:D:517:DG:C8	2.38	0.58
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.69	0.58
1:A:215:PRO:HG3	1:B:277:ASP:OD2	2.04	0.58
1:B:166:MET:HG3	1:B:244:LEU:HD11	1.84	0.58
1:A:136:LYS:HZ1	1:A:137:LEU:HD11	1.69	0.57
2:E:524:DT:C6	2:E:524:DT:H5'	2.39	0.57
1:B:208:GLY:O	1:B:209:LYS:HG3	2.05	0.57
1:B:141:LEU:HB2	1:B:294:PHE:HE1	1.67	0.57
1:B:250:ALA:HB1	1:B:255:THR:HG21	1.86	0.57
2:E:524:DT:H6	2:E:524:DT:H5'	1.69	0.57
1:B:167:PHE:HZ	1:B:317:ASN:O	1.88	0.57
2:C:518:DT:H2"	2:C:519:DG:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:HB	1:A:265:LYS:HG3	1.86	0.57
1:A:164:ARG:O	1:A:244:LEU:N	2.33	0.57
1:A:283:ALA:C	1:A:285:SER:HA	2.25	0.56
1:A:316:ASP:HB3	1:A:325:ARG:NE	2.19	0.56
2:F:503:DT:C4	2:F:504:DT:H73	2.40	0.56
1:A:218:ARG:NH1	1:A:218:ARG:HG2	2.17	0.56
1:A:271:HIS:CD2	1:A:291:VAL:HG22	2.40	0.56
1:B:287:SER:HB2	1:B:288:ASN:HA	1.86	0.56
1:A:170:LEU:HD23	1:A:187:VAL:HG21	1.87	0.56
1:B:322:LYS:HG2	1:B:325:ARG:HH22	1.70	0.56
2:E:518:DT:H2"	2:E:519:DG:C8	2.40	0.56
1:A:303:THR:HG21	2:E:504:DT:H2'	1.86	0.56
1:A:231:HIS:CA	1:A:234:ARG:HG3	2.26	0.56
1:A:167:PHE:HZ	1:A:317:ASN:O	1.89	0.56
1:B:269:ARG:HG3	1:B:293:THR:HG22	1.88	0.56
1:A:140:ALA:O	1:A:172:PHE:HB2	2.04	0.55
1:A:160:THR:HG22	1:A:162:GLN:H	1.71	0.55
1:B:316:ASP:HA	1:B:325:ARG:NE	2.21	0.55
1:A:217:ASN:OD1	1:A:218:ARG:N	2.39	0.55
1:A:312:GLN:OE1	1:A:325:ARG:NH1	2.38	0.55
1:B:165:ARG:HD3	1:B:241:LYS:HA	1.88	0.55
1:A:150:PHE:HE1	1:A:314:LYS:HG2	1.70	0.55
1:B:150:PHE:CE1	1:B:314:LYS:HG2	2.40	0.55
2:D:510:DC:H2"	2:D:511:DC:H5"	1.86	0.55
2:D:501:DA:H8	2:D:501:DA:HO5'	1.53	0.55
1:B:140:ALA:O	1:B:172:PHE:HB2	2.07	0.55
1:B:252:ASN:N	1:B:252:ASN:ND2	2.55	0.55
1:B:183:TYR:HD1	1:B:274:GLU:HG2	1.70	0.55
1:B:227:ASN:OD1	1:B:228:THR:N	2.40	0.55
1:B:218:ARG:HH21	1:B:259:VAL:CG1	2.16	0.54
2:F:503:DT:C2	2:F:504:DT:C5	2.96	0.54
1:A:316:ASP:O	1:A:322:LYS:NZ	2.23	0.54
1:A:200:GLN:O	1:A:203:LYS:N	2.41	0.54
1:A:198:ARG:HD3	2:E:503:DT:OP1	2.08	0.54
1:A:182:HIS:HB3	1:A:228:THR:HA	1.91	0.53
1:A:254:VAL:HA	1:B:255:THR:O	2.08	0.53
1:A:188:ASP:HB2	1:A:217:ASN:OD1	2.07	0.53
1:A:232:TRP:CE3	1:A:232:TRP:HA	2.43	0.53
2:C:518:DT:H3	2:D:507:DA:H61	1.55	0.53
1:B:293:THR:O	1:B:294:PHE:HD2	1.92	0.53
2:C:501:DA:H2"	2:C:502:DA:H5'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:OD1	1:A:228:THR:N	2.42	0.53
1:B:165:ARG:NE	2:D:515:DG:H5"	2.24	0.52
1:A:147:TRP:CD2	1:A:297:THR:HG22	2.44	0.52
1:A:199:TYR:CD2	1:A:306:GLN:HB3	2.44	0.52
1:B:166:MET:CG	1:B:244:LEU:HD11	2.39	0.52
1:B:188:ASP:CB	1:B:217:ASN:HD21	2.08	0.52
1:B:270:LEU:O	1:B:292:PHE:HB2	2.09	0.52
1:A:293:THR:O	1:A:294:PHE:HD2	1.92	0.52
2:C:516:DT:H2"	2:C:517:DG:H8	1.73	0.52
1:B:316:ASP:HA	1:B:325:ARG:NH2	2.24	0.51
1:A:214:MET:HB3	1:A:215:PRO:C	2.29	0.51
1:A:289:THR:HG22	1:B:286:ALA:HB3	1.91	0.51
1:B:159:ILE:HD13	1:B:246:ASN:HB3	1.92	0.51
1:A:150:PHE:CE1	1:A:314:LYS:HG2	2.45	0.50
1:B:192:VAL:HG21	1:B:298:GLN:OE1	2.11	0.50
1:B:234:ARG:HH11	1:B:234:ARG:HG3	1.76	0.50
1:A:316:ASP:OD1	1:A:317:ASN:N	2.44	0.50
1:A:256:GLN:HB3	1:B:253:ASN:OD1	2.12	0.50
1:B:254:VAL:HG12	1:B:254:VAL:O	2.11	0.50
1:B:150:PHE:HE1	1:B:314:LYS:HG2	1.76	0.50
1:A:137:LEU:H	1:A:176:GLY:HA3	1.77	0.50
1:A:159:ILE:HD13	1:A:246:ASN:HB3	1.94	0.49
1:B:185:MET:CG	1:B:272:ILE:HG22	2.42	0.49
1:B:262:SER:OG	1:B:263:LEU:HG	2.12	0.49
2:F:501:DA:H8	2:F:501:DA:HO5'	1.61	0.48
1:B:287:SER:CB	1:B:288:ASN:HA	2.43	0.48
2:F:510:DC:H2"	2:F:511:DC:H6	1.79	0.48
1:A:136:LYS:HZ2	1:A:137:LEU:HD11	1.75	0.48
1:A:188:ASP:OD1	1:A:271:HIS:CE1	2.66	0.48
1:B:165:ARG:HH21	2:D:515:DG:C5'	2.27	0.48
2:D:516:DT:C2'	2:D:517:DG:C8	2.97	0.48
2:F:514:DG:H2"	2:F:515:DG:H8	1.76	0.48
1:A:295:GLN:HG3	1:A:298:GLN:HE21	1.79	0.48
1:B:218:ARG:NH2	1:B:259:VAL:HG11	2.20	0.48
1:A:141:LEU:HA	1:A:172:PHE:HB3	1.96	0.48
1:A:245:THR:HG23	1:A:259:VAL:HG23	1.95	0.48
2:F:516:DT:H2"	2:F:517:DG:C8	2.49	0.48
1:A:177:LEU:HB2	1:A:183:TYR:CZ	2.48	0.47
1:A:154:GLN:HG3	1:A:204:TRP:NE1	2.28	0.47
1:A:141:LEU:HD22	1:A:294:PHE:CD1	2.49	0.47
1:A:217:ASN:O	1:A:218:ARG:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:504:DT:H2"	2:F:505:DT:O4'	2.15	0.47
1:B:147:TRP:CD2	1:B:297:THR:HG22	2.49	0.47
1:A:199:TYR:C	1:A:200:GLN:HE21	2.17	0.47
1:A:222:HIS:ND1	1:A:223:PRO:HD2	2.30	0.47
1:A:154:GLN:HG2	1:A:154:GLN:O	2.15	0.47
2:D:518:DT:H2"	2:D:519:DG:C8	2.50	0.46
1:A:295:GLN:O	1:A:298:GLN:HG3	2.15	0.46
1:A:178:GLU:N	1:A:183:TYR:OH	2.41	0.46
1:B:160:THR:HG22	1:B:162:GLN:N	2.30	0.46
2:F:512:DT:H2"	2:F:513:DA:H5'	1.96	0.46
1:A:172:PHE:CZ	1:A:270:LEU:HD13	2.51	0.46
1:A:276:ASN:CG	1:A:277:ASP:H	2.19	0.46
1:B:274:GLU:H	1:B:288:ASN:ND2	2.11	0.46
2:C:501:DA:HO5'	2:C:501:DA:H8	1.60	0.46
1:B:165:ARG:HH21	2:D:515:DG:H5"	1.80	0.46
1:B:177:LEU:HD11	1:B:233:MET:HG3	1.98	0.46
1:A:254:VAL:HG12	1:A:254:VAL:O	2.16	0.45
1:B:220:TYR:CG	1:B:242:LEU:HG	2.50	0.45
1:B:283:ALA:C	1:B:285:SER:H	2.20	0.45
1:B:295:GLN:HG3	1:B:298:GLN:HE21	1.81	0.45
2:D:512:DT:H2"	2:D:513:DA:H5'	1.97	0.45
1:A:188:ASP:CB	1:A:217:ASN:HD21	2.30	0.45
1:A:191:LEU:HD12	1:A:266:TYR:CE1	2.51	0.45
1:B:150:PHE:HB3	1:B:155:THR:HG23	1.99	0.45
1:B:303:THR:HG21	2:C:504:DT:H2'	1.98	0.45
1:A:153:HIS:HB3	1:A:309:GLU:OE2	2.16	0.45
1:B:272:ILE:HG12	1:B:290:HIS:CE1	2.51	0.45
2:C:511:DC:H2'	2:C:512:DT:C6	2.51	0.45
1:A:218:ARG:NH1	1:B:226:PRO:HD3	2.32	0.45
1:B:322:LYS:CB	1:B:325:ARG:HH12	2.26	0.45
1:A:184:ARG:O	1:A:272:ILE:HA	2.17	0.45
1:A:177:LEU:HD11	1:A:233:MET:HG3	1.98	0.45
1:A:149:LYS:O	1:A:153:HIS:CD2	2.70	0.45
1:B:186:PHE:HA	1:B:221:VAL:HA	1.99	0.45
1:B:245:THR:HG23	1:B:259:VAL:HG23	1.99	0.45
1:A:232:TRP:HE3	1:A:232:TRP:HA	1.82	0.44
2:F:504:DT:C6	2:F:505:DT:H72	2.53	0.44
1:A:200:GLN:CA	1:A:200:GLN:HE21	2.29	0.44
1:B:147:TRP:CE2	1:B:297:THR:HG22	2.52	0.44
1:B:190:VAL:O	1:B:267:GLN:N	2.49	0.44
1:B:218:ARG:HB2	1:B:218:ARG:CZ	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD22	1:A:266:TYR:CZ	2.52	0.44
1:B:322:LYS:CG	1:B:325:ARG:HH22	2.31	0.44
1:A:218:ARG:CG	1:A:218:ARG:NH1	2.81	0.43
1:A:165:ARG:HA	1:A:242:LEU:O	2.18	0.43
1:B:191:LEU:HB3	1:B:214:MET:O	2.19	0.43
1:B:317:ASN:O	1:B:319:PRO:HD3	2.19	0.43
1:B:172:PHE:CZ	1:B:270:LEU:HD13	2.54	0.43
1:B:228:THR:OG1	1:B:231:HIS:N	2.42	0.43
1:B:158:ILE:HA	1:B:302:VAL:O	2.18	0.43
2:E:501:DA:H8	2:E:501:DA:HO5'	1.65	0.43
1:B:209:LYS:O	1:B:211:GLU:HG2	2.18	0.43
1:B:174:VAL:HG11	1:B:185:MET:HE1	2.00	0.42
1:B:318:ASN:HA	1:B:319:PRO:HD3	1.77	0.42
1:A:193:ASP:OD1	1:A:194:GLN:HG2	2.20	0.42
1:B:215:PRO:HB2	1:B:216:GLY:H	1.47	0.42
1:A:295:GLN:C	1:A:297:THR:H	2.23	0.42
2:F:523:DT:H1'	2:F:524:DT:H5"	2.02	0.42
1:B:154:GLN:NE2	1:B:307:ASN:HD22	2.16	0.42
2:E:523:DT:C2	2:E:524:DT:H72	2.54	0.42
1:B:305:TYR:OH	1:B:314:LYS:HD2	2.20	0.42
1:A:169:PHE:CG	1:A:240:GLY:HA2	2.54	0.42
1:A:189:VAL:CG1	1:A:258:ILE:HG21	2.50	0.42
1:B:178:GLU:HA	1:B:179:PRO:HD3	1.86	0.42
1:A:153:HIS:N	1:A:153:HIS:CD2	2.87	0.42
1:B:146:LEU:HD23	1:B:168:PRO:HB3	2.00	0.42
1:B:310:ILE:HG22	1:B:311:THR:N	2.34	0.42
1:B:305:TYR:CZ	1:B:314:LYS:HD2	2.55	0.42
2:F:511:DC:H2'	2:F:512:DT:C6	2.55	0.42
1:B:234:ARG:NH1	1:B:234:ARG:HG3	2.34	0.42
1:A:253:ASN:O	1:A:255:THR:HG23	2.19	0.42
1:B:199:TYR:CZ	1:B:202:GLY:HA2	2.54	0.42
1:B:253:ASN:CG	1:B:254:VAL:N	2.73	0.42
1:B:291:VAL:O	1:B:292:PHE:HD1	2.02	0.42
1:B:185:MET:HG2	1:B:272:ILE:HG22	2.02	0.41
2:E:508:DC:H2"	2:E:509:DA:C8	2.55	0.41
1:B:141:LEU:HD22	1:B:294:PHE:CD1	2.54	0.41
2:F:510:DC:H2"	2:F:511:DC:C6	2.56	0.41
1:A:215:PRO:HG3	1:B:277:ASP:CG	2.40	0.41
1:A:177:LEU:C	1:A:177:LEU:HD12	2.40	0.41
1:A:160:THR:HG22	1:A:162:GLN:N	2.36	0.41
1:B:232:TRP:HA	1:B:232:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:509:DA:H1'	2:D:510:DC:H5'	2.02	0.41
2:D:510:DC:H2"	2:D:511:DC:C5'	2.49	0.41
1:A:317:ASN:O	1:A:319:PRO:HD3	2.20	0.41
1:B:295:GLN:O	1:B:298:GLN:HG3	2.21	0.41
1:B:141:LEU:HA	1:B:172:PHE:HB3	2.03	0.41
1:B:276:ASN:OD1	1:B:276:ASN:N	2.36	0.41
1:A:142:SER:O	1:A:143:ASN:HB2	2.20	0.41
1:B:307:ASN:OD1	1:B:309:GLU:N	2.45	0.41
1:A:189:VAL:CG2	1:A:266:TYR:HB3	2.51	0.41
1:A:254:VAL:O	1:B:254:VAL:HG13	2.21	0.40
1:A:199:TYR:OH	1:A:307:ASN:HB2	2.21	0.40
1:A:274:GLU:HG3	1:A:288:ASN:ND2	2.36	0.40
1:B:272:ILE:HG13	1:B:272:ILE:O	2.21	0.40
1:A:191:LEU:HD13	1:A:216:GLY:H	1.86	0.40
1:A:322:LYS:HD3	1:A:322:LYS:HA	1.82	0.40
1:A:275:VAL:HG11	1:B:215:PRO:HG2	2.03	0.40
1:B:295:GLN:C	1:B:297:THR:H	2.24	0.40
1:A:179:PRO:O	1:A:228:THR:OG1	2.39	0.40
1:B:189:VAL:CG1	1:B:258:ILE:HG21	2.50	0.40
1:A:217:ASN:CB	1:B:184:ARG:HH22	2.27	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	190/204 (93%)	153 (80%)	30 (16%)	7 (4%)	4 15
1	B	190/204 (93%)	156 (82%)	26 (14%)	8 (4%)	3 12
All	All	380/408 (93%)	309 (81%)	56 (15%)	15 (4%)	4 14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	MET
1	A	215	PRO
1	A	234	ARG
1	B	154	GLN
1	B	213	SER
1	B	214	MET
1	B	215	PRO
1	B	284	CYS
1	A	154	GLN
1	A	212	GLY
1	A	236	GLU
1	A	280	PRO
1	B	217	ASN
1	B	212	GLY
1	B	201	SER

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	169/179 (94%)	154 (91%)	15 (9%)	12	34
1	B	169/179 (94%)	153 (90%)	16 (10%)	11	30
All	All	338/358 (94%)	307 (91%)	31 (9%)	11	32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	155	THR
1	A	172	PHE
1	A	178	GLU
1	A	184	ARG
1	A	187	VAL
1	A	193	ASP
1	A	198	ARG
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	218	ARG
1	A	244	LEU
1	A	270	LEU
1	A	271	HIS
1	A	274	GLU
1	A	310	ILE
1	B	146	LEU
1	B	165	ARG
1	B	172	PHE
1	B	182	HIS
1	B	187	VAL
1	B	193	ASP
1	B	199	TYR
1	B	200	GLN
1	B	228	THR
1	B	244	LEU
1	B	248	LYS
1	B	252	ASN
1	B	265	LYS
1	B	270	LEU
1	B	271	HIS
1	B	310	ILE

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

Mol	Chain	Res	Type
1	A	154	GLN
1	A	182	HIS
1	A	194	GLN
1	A	200	GLN
1	A	261	GLN
1	A	276	ASN
1	A	290	HIS
1	B	154	GLN
1	B	252	ASN
1	B	256	GLN

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	192/204 (94%)	0.52	21 (10%) 7 5	75, 115, 211, 278	0
1	B	192/204 (94%)	0.58	21 (10%) 7 5	76, 115, 211, 304	0
2	C	24/24 (100%)	-0.47	0 100 100	89, 125, 180, 188	0
2	D	24/24 (100%)	-0.46	0 100 100	94, 127, 176, 178	0
2	E	24/24 (100%)	-0.31	1 (4%) 40 36	100, 134, 178, 200	0
2	F	24/24 (100%)	-0.22	1 (4%) 40 36	99, 136, 224, 259	0
All	All	480/504 (95%)	0.37	44 (9%) 11 8	75, 121, 211, 304	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	PRO	10.2
1	B	282	ALA	9.0
1	A	282	ALA	8.9
1	B	283	ALA	7.4
2	F	501	DA	7.3
1	A	275	VAL	5.2
1	A	216	GLY	5.2
1	B	285	SER	5.1
1	B	215	PRO	5.0
1	B	137	LEU	4.8
1	B	278	GLY	4.7
1	B	251	SER	4.5
1	A	176	GLY	4.3
1	A	177	LEU	4.2
1	A	291	VAL	4.0
1	A	280	PRO	3.8
1	A	182	HIS	3.6
1	B	279	GLU	3.6
1	B	211	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	140	ALA	3.4
1	A	279	GLU	3.3
1	B	260	LEU	3.3
1	A	293	THR	3.1
1	A	324	PHE	3.1
1	A	278	GLY	3.1
1	B	185	MET	3.0
1	B	321	ALA	3.0
1	B	138	ARG	2.9
1	A	180	THR	2.8
1	B	324	PHE	2.8
1	A	217	ASN	2.7
1	A	174	VAL	2.6
1	A	320	PHE	2.6
1	A	294	PHE	2.5
1	B	209	LYS	2.5
1	A	138	ARG	2.4
1	B	327	ASN	2.4
1	B	263	LEU	2.4
1	A	170	LEU	2.4
1	A	248	LYS	2.3
1	B	281	GLU	2.2
1	B	174	VAL	2.2
2	E	524	DT	2.1
1	B	140	ALA	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.