



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 PM UTC

PDB ID : 5T1J / pdb_00005t1j
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

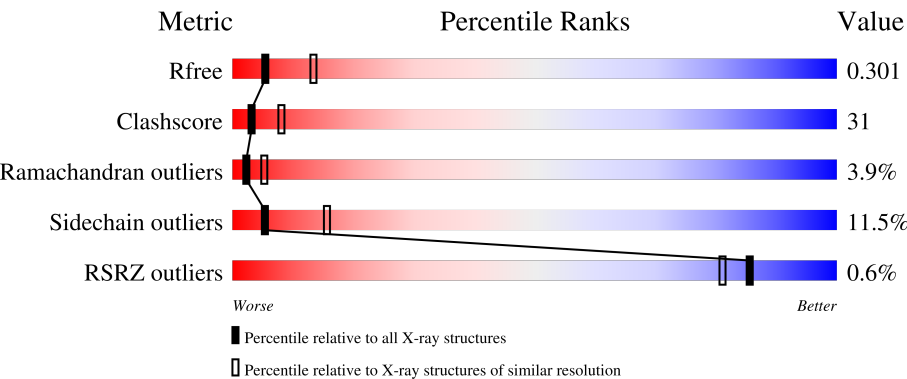
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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.



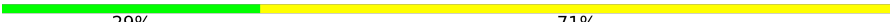
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	% 39% 42% 12% 6%
1	B	204	35% 49% 10% 6%
2	C	24	46% 54%
2	D	24	42% 58%
2	E	24	54% 46%

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Mol	Chain	Length	Quality of chain
2	F	24	 29% 71%

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

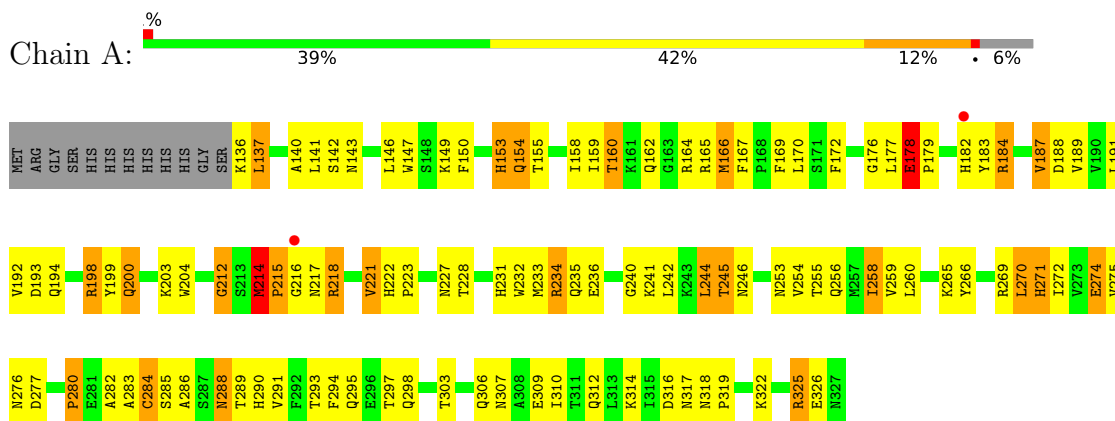
- Molecule 2 is a DNA chain called DNA.

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

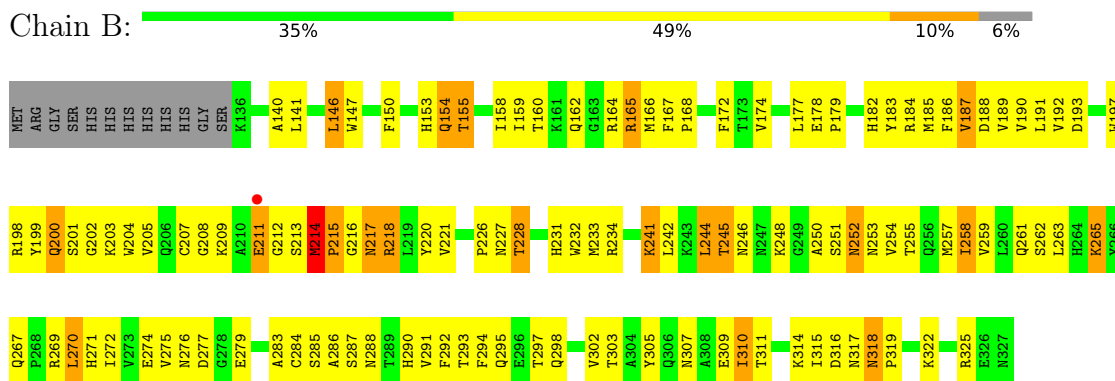
3 Residue-property plots

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.

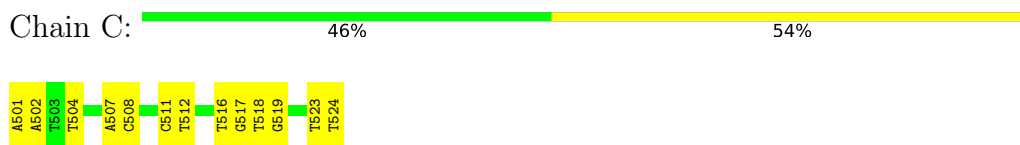
• Molecule 1: T-box transcription factor TBX21



• Molecule 1: T-box transcription factor TBX21



• Molecule 2: DNA



• Molecule 2: DNA





● Molecule 2: DNA



● Molecule 2: DNA



4 Data and refinement statistics

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) 88.0 (43.70-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.266 , 0.294 0.269 , 0.301	Depositor DCC
R_{free} test set	1155 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 148.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.81	1/1594 (0.1%)	1.36	14/2157 (0.6%)
1	B	0.76	0/1594	1.25	8/2157 (0.4%)
2	C	0.47	0/548	0.76	0/844
2	D	0.47	0/548	0.74	0/844
2	E	0.54	0/548	0.75	0/844
2	F	0.45	0/548	0.73	0/844
All	All	0.68	1/5380 (0.0%)	1.10	22/7690 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	VAL	CA-CB	6.73	1.62	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	MET	C-N-CD	-13.72	90.42	120.60
1	A	214	MET	CA-C-N	11.92	155.61	127.00
1	A	214	MET	C-N-CA	11.92	155.61	127.00
1	A	318	ASN	CA-C-N	9.17	128.91	119.56
1	A	318	ASN	C-N-CA	9.17	128.91	119.56
1	A	284	CYS	N-CA-C	7.34	121.50	112.54
1	B	318	ASN	CA-C-N	6.74	126.44	119.56
1	B	318	ASN	C-N-CA	6.74	126.44	119.56
1	B	218	ARG	N-CA-C	-6.57	97.54	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASN	N-CA-C	6.25	119.66	109.59
1	A	290	HIS	N-CA-C	6.20	119.24	108.76
1	B	211	GLU	N-CA-C	5.99	122.64	112.99
1	A	245	THR	N-CA-C	5.85	115.96	108.24
1	B	245	THR	N-CA-C	5.78	116.18	108.38
1	A	178	GLU	CA-C-N	5.76	124.96	118.97
1	A	178	GLU	C-N-CA	5.76	124.96	118.97
1	A	166	MET	N-CA-C	5.25	117.06	110.24
1	A	326	GLU	N-CA-C	-5.24	106.84	113.18
1	B	279	GLU	CA-C-N	5.14	126.27	119.84
1	B	279	GLU	C-N-CA	5.14	126.27	119.84
1	B	153	HIS	N-CA-C	-5.11	106.79	112.57
1	A	325	ARG	N-CA-C	5.01	120.33	114.62

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

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	122	0
1	B	1553	0	1512	126	0
2	C	489	0	274	11	0
2	D	489	0	274	15	0
2	E	489	0	274	10	0
2	F	489	0	274	17	0
All	All	5062	0	4120	275	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 31.

All (275) 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
1:A:231:HIS:HA	1:A:234:ARG:HG3	1.41	1.00
1:B:251:SER:C	1:B:252:ASN:HD22	1.75	0.95
1:A:154:GLN:HG3	1:A:204:TRP:CD1	2.04	0.92
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:HE21	1:A:200:GLN:N	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:187:VAL:HG23	1:A:270:LEU:HB2	1.66	0.76
1:A:218:ARG:HG2	1:A:218:ARG:HH11	1.50	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:HD22	1:B:252:ASN:N	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:A:283:ALA:C	1:A:285:SER:HA	2.25	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:HG2	1:A:184:ARG:HH11	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:H5'	2:E:524:DT:C6	2.39	0.57
1:B:141:LEU:HB2	1:B:294:PHE:HE1	1.67	0.57
1:B:208:GLY:O	1:B:209:LYS:HG3	2.05	0.57
1:B:250:ALA:HB1	1:B:255:THR:HG21	1.86	0.57
2:E:524:DT:H5'	2:E:524:DT:H6	1.69	0.57
1:B:167:PHE:HZ	1:B:317:ASN:O	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:518:DT:H2''	2:C:519:DG:C8	2.40	0.57
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: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:HG2	1:A:218:ARG:NH1	2.17	0.56
1:A:170:LEU:HD23	1:A:187:VAL:HG21	1.87	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: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:214:MET:HB3	1:A:215:PRO:C	2.29	0.56
1:A:303:THR:HG21	2:E:504:DT:H2'	1.86	0.56
2:D:501:DA:H8	2:D:501:DA:HO5'	1.52	0.56
1:A:167:PHE:HZ	1:A:317:ASN:O	1.89	0.56
1:A:231:HIS:CA	1:A:234:ARG:HG3	2.26	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
1:B:140:ALA:O	1:B:172:PHE:HB2	2.07	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:HA	1:A:232:TRP:CE3	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:A:214:MET:HE2	1:B:226:PRO:HB3	1.91	0.52
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
1:A:199:TYR:C	1:A:200:GLN:HE21	2.17	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: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:B:252:ASN:N	1:B:252:ASN:ND2	2.55	0.51
1:A:150:PHE:CE1	1:A:314:LYS:HG2	2.45	0.50
1:A:276:ASN:CG	1:A:277:ASP:H	2.19	0.50
1:B:192:VAL:HG21	1:B:298:GLN:OE1	2.11	0.50
1:B:234:ARG:HG3	1:B:234:ARG:HH11	1.76	0.50
1:A:316:ASP:OD1	1:A:317:ASN:N	2.44	0.50
1:B:283:ALA:C	1:B:285:SER:H	2.20	0.50
1:A:256:GLN:HB3	1:B:253:ASN:OD1	2.12	0.50
1:B:150:PHE:HE1	1:B:314:LYS:HG2	1.76	0.50
1:B:254:VAL:HG12	1:B:254:VAL:O	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD22	1:A:294:PHE:CD1	2.49	0.47
1:A:154:GLN:HG3	1:A:204:TRP:NE1	2.28	0.47
1:A:217:ASN:O	1:A:218:ARG:HG2	2.13	0.47
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:295:GLN:C	1:A:297:THR:H	2.23	0.47
1:A:222:HIS:ND1	1:A:223:PRO:HD2	2.30	0.47
2:F:501:DA:HO5'	2:F:501:DA:H8	1.63	0.47
1:A:154:GLN:O	1:A:154:GLN:HG2	2.15	0.47
1:A:177:LEU:C	1:A:177:LEU:HD12	2.40	0.47
2:D:518:DT:H2''	2:D:519:DG:C8	2.50	0.46
1:B:253:ASN:CG	1:B:254:VAL:N	2.73	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:215:PRO:HG3	1:B:277:ASP:CG	2.40	0.46
1:A:172:PHE:CZ	1:A:270:LEU:HD13	2.51	0.46
1:B:274:GLU:H	1:B:288:ASN:ND2	2.11	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:160:THR:O	1:A:245:THR:OG1	2.33	0.45
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: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:295:GLN:C	1:B:297:THR:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TRP:HA	1:A:232:TRP:HE3	1.82	0.44
2:F:504:DT:C6	2:F:505:DT:H72	2.53	0.44
1:A:200:GLN:HE21	1:A:200:GLN:CA	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:CZ	1:B:218:ARG:HB2	2.46	0.44
1:A:212:GLY:C	1:A:214:MET:N	2.75	0.44
1:A:260:LEU:HD22	1:A:266:TYR:CZ	2.52	0.44
1:B:177:LEU:HD12	1:B:177:LEU:C	2.42	0.44
1:B:322:LYS:CG	1:B:325:ARG:HH22	2.31	0.44
2:C:501:DA:HO5'	2:C:501:DA:H8	1.62	0.44
1:A:218:ARG:NH1	1:A:218:ARG:CG	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:A:280:PRO:C	1:A:282:ALA:HA	2.44	0.43
1:B:158:ILE:HA	1:B:302:VAL:O	2.18	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
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:CD2	1:A:153:HIS:N	2.87	0.42
1:B:146:LEU:HD23	1:B:168:PRO:HB3	2.00	0.42
1:B:305:TYR:CZ	1:B:314:LYS:HD2	2.55	0.42
1:B:310:ILE:HG22	1:B:311:THR:N	2.34	0.42
2:F:511:DC:H2'	2:F:512:DT:C6	2.55	0.42
1:B:234:ARG:HG3	1:B:234:ARG:NH1	2.34	0.42
1:A:194:GLN:HE22	1:B:277:ASP:CG	2.28	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:291:VAL:O	1:B:292:PHE:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:160:THR:HG22	1:A:162:GLN:N	2.36	0.41
1:B:232:TRP:CE3	1:B:232:TRP:HA	2.56	0.41
1:B:270:LEU:C	1:B:270:LEU:HD23	2.45	0.41
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:A:142:SER:O	1:A:143:ASN:HB2	2.20	0.41
1:B:141:LEU:HA	1:B:172:PHE:HB3	2.03	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:199:TYR:OH	1:A:307:ASN:HB2	2.21	0.40
1:A:212:GLY:C	1:A:214:MET:H	2.29	0.40
1:A:254:VAL:O	1:B:254:VAL:HG13	2.21	0.40
1:A:214:MET:HE3	1:B:275:VAL:CG2	2.51	0.40
1:A:274:GLU:HG3	1:A:288:ASN:ND2	2.36	0.40
1:B:272:ILE:O	1:B:272:ILE:HG13	2.21	0.40
1:A:191:LEU:HD13	1:A:216:GLY:H	1.86	0.40
1:A:275:VAL:HG11	1:B:215:PRO:HG2	2.03	0.40
1:A:322:LYS:HD3	1:A:322:LYS:HA	1.82	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
1:A:276:ASN:CG	1:A:277:ASP:N	2.79	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%)	2	6
1	B	190/204 (93%)	156 (82%)	26 (14%)	8 (4%)	2	5
All	All	380/408 (93%)	309 (81%)	56 (15%)	15 (4%)	2	5

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 ⓘ

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%)	150 (89%)	19 (11%)	6	16
1	B	169/179 (94%)	149 (88%)	20 (12%)	5	14
All	All	338/358 (94%)	299 (88%)	39 (12%)	5	15

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	146	LEU
1	A	153	HIS
1	A	155	THR
1	A	160	THR
1	A	178	GLU
1	A	184	ARG
1	A	187	VAL
1	A	198	ARG
1	A	200	GLN
1	A	218	ARG
1	A	221	VAL
1	A	241	LYS
1	A	244	LEU
1	A	258	ILE
1	A	270	LEU
1	A	271	HIS
1	A	274	GLU
1	A	310	ILE
1	B	146	LEU
1	B	155	THR
1	B	165	ARG
1	B	187	VAL
1	B	193	ASP
1	B	200	GLN
1	B	205	VAL
1	B	214	MET
1	B	228	THR
1	B	241	LYS
1	B	244	LEU
1	B	248	LYS
1	B	252	ASN
1	B	258	ILE
1	B	261	GLN
1	B	265	LYS
1	B	270	LEU
1	B	271	HIS
1	B	276	ASN
1	B	310	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	154	GLN
1	A	194	GLN
1	A	200	GLN
1	A	261	GLN
1	A	267	GLN
1	A	276	ASN
1	A	290	HIS
1	A	298	GLN
1	B	154	GLN
1	B	247	ASN
1	B	252	ASN
1	B	256	GLN
1	B	290	HIS
1	B	317	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 oligosaccharides 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	192/204 (94%)	-0.18	2 (1%) 79 74	75, 115, 211, 278	0
1	B	192/204 (94%)	-0.22	1 (0%) 87 83	76, 115, 211, 304	0
2	C	24/24 (100%)	-0.38	0 100 100	89, 125, 180, 188	0
2	D	24/24 (100%)	-0.28	0 100 100	94, 127, 176, 178	0
2	E	24/24 (100%)	-0.32	0 100 100	100, 134, 178, 200	0
2	F	24/24 (100%)	-0.19	0 100 100	99, 136, 224, 259	0
All	All	480/504 (95%)	-0.22	3 (0%) 85 81	75, 121, 211, 304	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	HIS	3.5
1	A	216	GLY	2.7
1	B	211	GLU	2.1

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 oligosaccharides 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.