



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:53 PM GMT

PDB ID : 1VOL  
Title : TFIIB (HUMAN CORE DOMAIN)/TBP (A.THALIANA)/TATA ELEMENT TERNARY COMPLEX  
Authors : Nikolov, D.B.; Chen, H.; Halay, E.D.; Usheva, A.U.; Hisatake, K.; Lee, D.K.; Roeder, R.G.; Burley, S.K.  
Deposited on : 1996-04-29  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

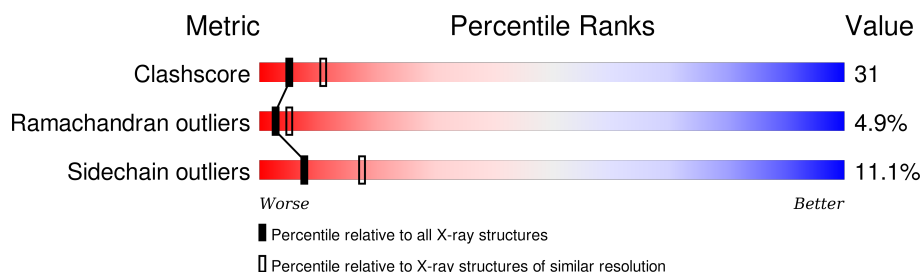
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	16	
2	D	16	
3	A	204	
4	B	200	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3715 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 DNA (5'-D(\*GP\*GP\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*GP\*GP\*GP\*CP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	16	Total	C	N	O	P	0	0	0
			332	158	67	92	15			

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*AP\*GP\*CP\*CP\*CP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*GP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	P	0	0	0
			318	154	53	96	15			

- Molecule 3 is a protein called PROTEIN (TRANSCRIPTION FACTOR IIB (TFIIB)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	204	Total	C	N	O	S	0	0	0
			1590	1002	285	291	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	LYS	ILE	CONFLICT	UNP Q00403
A	143	ARG	LYS	CONFLICT	UNP Q00403
A	145	ALA	VAL	CONFLICT	UNP Q00403

- Molecule 4 is a protein called PROTEIN (TATA BINDING PROTEIN (TBP)).

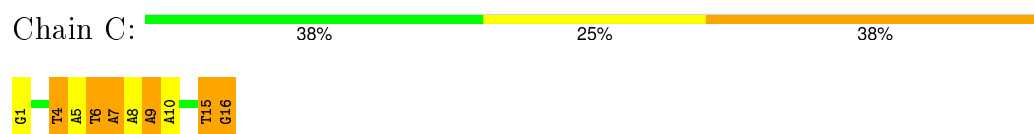
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	187	Total	C	N	O	S	0	0	0
			1475	962	251	254	8			

### 3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*GP\*GP\*GP\*CP\*TP\*G)-3')



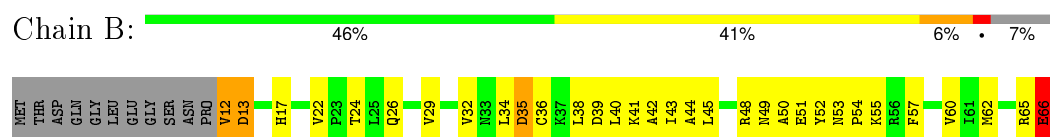
- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*CP\*CP\*CP\*TP\*TP\*TP\*TP\*AP\*TP\*AP\*GP\*CP\*C)-3')

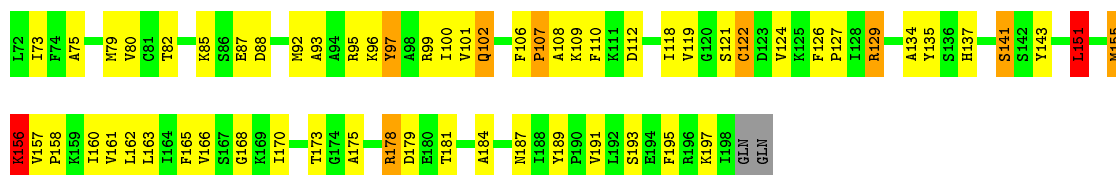


- Molecule 3: PROTEIN (TRANSCRIPTION FACTOR IIB (TFIIB))



- Molecule 4: PROTEIN (TATA BINDING PROTEIN (TBP))





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.90 Å 78.00 Å 134.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.215 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 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	1.57	3/374 (0.8%)	1.84	9/577 (1.6%)
2	D	1.60	1/354 (0.3%)	2.42	26/543 (4.8%)
3	A	0.64	0/1614	0.84	1/2175 (0.0%)
4	B	0.73	1/1505 (0.1%)	0.91	4/2026 (0.2%)
All	All	0.92	5/3847 (0.1%)	1.25	40/5321 (0.8%)

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
3	A	0	1
4	B	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	122	CYS	CB-SG	-6.64	1.71	1.82
1	C	6	DT	C4'-O4'	-5.58	1.39	1.45
2	D	108	DT	C4'-C3'	-5.41	1.47	1.52
1	C	15	DT	C5-C7	5.39	1.53	1.50
1	C	7	DA	C4'-O4'	-5.01	1.40	1.45

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	DT	O4'-C4'-C3'	-11.78	98.93	106.00
2	D	101	DC	O4'-C1'-N1	11.63	116.14	108.00
2	D	115	DC	O4'-C1'-C2'	-11.27	96.88	105.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	104	DC	O4'-C1'-N1	9.78	114.85	108.00
1	C	7	DA	O4'-C4'-C3'	-9.35	100.39	106.00
1	C	8	DA	O4'-C4'-C3'	-8.92	100.65	106.00
2	D	103	DG	O4'-C4'-C3'	-8.01	101.19	106.00
2	D	107	DT	C6-C5-C7	-7.63	118.32	122.90
2	D	113	DA	O4'-C1'-C2'	-7.34	100.03	105.90
2	D	116	DC	O4'-C1'-N1	7.02	112.91	108.00
2	D	105	DC	O4'-C4'-C3'	-6.87	101.75	104.50
2	D	101	DC	C2-N3-C4	-6.77	116.51	119.90
2	D	110	DT	C6-C5-C7	-6.71	118.88	122.90
2	D	108	DT	O4'-C1'-C2'	-6.46	100.73	105.90
1	C	15	DT	O4'-C1'-C2'	-6.30	100.86	105.90
1	C	8	DA	P-O3'-C3'	6.15	127.08	119.70
2	D	105	DC	O4'-C1'-N1	6.06	112.24	108.00
1	C	6	DT	C4-C5-C6	6.05	121.63	118.00
1	C	16	DG	C3'-C2'-C1'	-6.04	95.26	102.50
4	B	151	LEU	CA-CB-CG	5.91	128.90	115.30
2	D	108	DT	C4-C5-C6	5.86	121.52	118.00
2	D	107	DT	C1'-O4'-C4'	-5.83	104.27	110.10
2	D	104	DC	C4'-C3'-C2'	-5.71	97.96	103.10
1	C	9	DA	P-O3'-C3'	5.67	126.50	119.70
2	D	101	DC	C1'-O4'-C4'	-5.65	104.45	110.10
2	D	102	DA	O4'-C1'-N9	5.62	111.94	108.00
1	C	4	DT	C6-C5-C7	-5.62	119.53	122.90
2	D	111	DA	P-O3'-C3'	5.54	126.35	119.70
3	A	184	SER	N-CA-C	5.41	125.61	111.00
2	D	110	DT	C1'-O4'-C4'	-5.32	104.78	110.10
4	B	12	VAL	N-CA-C	5.32	125.36	111.00
2	D	109	DT	O4'-C1'-N1	-5.30	104.29	108.00
2	D	101	DC	P-O3'-C3'	5.24	125.99	119.70
2	D	109	DT	C6-C5-C7	-5.13	119.82	122.90
4	B	163	LEU	CA-CB-CG	5.13	127.10	115.30
2	D	112	DT	O4'-C4'-C3'	-5.10	102.46	104.50
2	D	109	DT	C4-C5-C6	5.06	121.04	118.00
2	D	105	DC	N1-C2-O2	5.05	121.93	118.90
4	B	112	ASP	N-CA-C	5.04	124.62	111.00
1	C	5	DA	C5'-C4'-C3'	-5.03	105.04	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	A	146	TYR	Sidechain
4	B	97	TYR	Sidechain
1	C	1	DG	Sidechain
2	D	112	DT	Sidechain

## 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	C	332	0	181	11	0
2	D	318	0	183	20	0
3	A	1590	0	1646	123	0
4	B	1475	0	1558	84	0
All	All	3715	0	3568	223	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 (223) 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)
3:A:116:ASN:HA	3:A:119:LYS:HD3	1.39	0.99
4:B:102:GLN:HG3	4:B:108:ALA:HB3	1.47	0.96
3:A:224:LEU:HD22	3:A:228:VAL:HG11	1.49	0.95
3:A:155:ALA:HB3	3:A:158:ALA:HB2	1.51	0.92
3:A:134:LYS:O	3:A:138:THR:HG22	1.76	0.86
1:C:15:DT:H2"	1:C:16:DG:N7	1.92	0.85
3:A:270:THR:OG1	3:A:273:GLU:HG3	1.78	0.84
3:A:131:PRO:HG2	3:A:133:ASN:OD1	1.84	0.77
3:A:175:ARG:HA	3:A:217:ARG:NH2	1.99	0.77
3:A:207:ASP:O	3:A:208:LEU:HB2	1.84	0.76
4:B:79:MET:HE1	4:B:97:TYR:HB3	1.66	0.76
3:A:176:THR:OG1	3:A:179:GLU:HG3	1.84	0.76
4:B:127:PRO:HB2	4:B:197:LYS:HE3	1.68	0.76
4:B:156:LYS:HG2	4:B:157:VAL:H	1.50	0.74
4:B:160:ILE:HG12	4:B:184:ALA:HB2	1.67	0.74
3:A:286:ARG:NH1	3:A:316:LEU:HD22	2.02	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:79:MET:CE	4:B:97:TYR:HB3	2.18	0.73
4:B:143:TYR:HB2	4:B:151:LEU:HD22	1.71	0.73
4:B:67:PRO:HG2	4:B:93:ALA:HB2	1.70	0.73
2:D:110:DT:O2	4:B:119:VAL:HG21	1.89	0.73
3:A:166:ILE:O	3:A:170:GLN:HG3	1.89	0.71
3:A:169:ARG:HG2	3:A:174:PRO:HB3	1.73	0.71
4:B:155:MET:HE1	4:B:187:ASN:HD22	1.55	0.71
3:A:155:ALA:HB3	3:A:158:ALA:CB	2.22	0.70
3:A:208:LEU:HG	4:B:135:TYR:CE2	2.25	0.70
4:B:12:VAL:O	4:B:13:ASP:HB2	1.92	0.70
4:B:17:HIS:CD2	4:B:22:VAL:HG22	2.26	0.70
4:B:124:VAL:HG23	4:B:168:GLY:O	1.93	0.69
3:A:266:ALA:O	3:A:268:LYS:HG3	1.92	0.69
4:B:156:LYS:H	4:B:156:LYS:HD3	1.55	0.69
2:D:108:DT:H2''	2:D:109:DT:O5'	1.91	0.69
3:A:226:LYS:HD2	3:A:226:LYS:O	1.94	0.68
3:A:289:TYR:CD2	3:A:316:LEU:HD12	2.28	0.68
3:A:130:LEU:HD22	3:A:134:LYS:HD2	1.75	0.68
3:A:168:CYS:SG	3:A:175:ARG:HD3	2.34	0.68
3:A:263:GLN:HA	3:A:268:LYS:HG2	1.76	0.67
4:B:29:VAL:HG22	4:B:82:THR:HG22	1.76	0.67
4:B:34:LEU:HA	4:B:109:LYS:O	1.95	0.66
2:D:103:DG:H2'	2:D:104:DC:C6	2.30	0.66
3:A:301:PRO:O	3:A:302:THR:HG23	1.95	0.66
3:A:264:ALA:HB1	3:A:306:PHE:CE1	2.31	0.66
3:A:143:ARG:HH11	3:A:143:ARG:HG3	1.62	0.65
3:A:208:LEU:O	3:A:209:ILE:HB	1.96	0.65
4:B:155:MET:HG3	4:B:162:LEU:HD11	1.79	0.65
4:B:155:MET:HB2	4:B:160:ILE:HD12	1.79	0.65
3:A:287:GLN:O	3:A:291:LEU:HG	1.98	0.64
4:B:52:TYR:HB2	4:B:60:VAL:HG22	1.78	0.63
1:C:7:DA:N3	4:B:173:THR:HG21	2.13	0.63
4:B:143:TYR:HB2	4:B:151:LEU:CD2	2.28	0.62
3:A:125:ALA:HB1	3:A:135:VAL:HG22	1.81	0.62
4:B:95:ARG:HE	4:B:99:ARG:NH2	1.96	0.62
3:A:116:ASN:O	3:A:119:LYS:HB2	2.01	0.60
3:A:168:CYS:SG	3:A:175:ARG:CD	2.89	0.60
4:B:127:PRO:HA	4:B:166:VAL:O	2.01	0.60
1:C:15:DT:H3	2:D:102:DA:H61	1.50	0.59
4:B:26:GLN:O	4:B:85:LYS:HE2	2.01	0.59
3:A:128:ILE:O	3:A:128:ILE:HD13	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:113:ALA:O	3:A:117:ALA:HB2	2.02	0.58
3:A:210:THR:O	3:A:213:ASP:HB2	2.04	0.58
3:A:115:MET:HB3	3:A:119:LYS:NZ	2.18	0.58
4:B:178:ARG:O	4:B:181:THR:HB	2.04	0.58
3:A:222:LEU:HD22	3:A:269:ARG:HG3	1.86	0.58
3:A:116:ASN:CA	3:A:119:LYS:HD3	2.26	0.57
4:B:50:ALA:HA	4:B:62:MET:HA	1.86	0.57
3:A:194:CYS:O	3:A:198:ILE:HG13	2.03	0.57
4:B:54:PRO:HG2	4:B:55:LYS:HE2	1.87	0.57
4:B:35:ASP:HB2	4:B:109:LYS:HB2	1.87	0.57
2:D:104:DC:H2'	2:D:105:DC:H6	1.68	0.57
4:B:40:LEU:CD2	4:B:75:ALA:HB2	2.34	0.56
3:A:149:LYS:NZ	3:A:149:LYS:HB2	2.21	0.56
3:A:275:GLY:CA	3:A:285:ILE:HD11	2.35	0.56
4:B:41:LYS:O	4:B:45:LEU:HD23	2.05	0.56
4:B:129:ARG:HH11	4:B:129:ARG:HG2	1.71	0.56
3:A:262:SER:OG	3:A:268:LYS:HA	2.06	0.56
3:A:305:LYS:O	3:A:306:PHE:HB2	2.06	0.56
4:B:40:LEU:HD12	4:B:60:VAL:CG2	2.36	0.56
3:A:239:ALA:HA	3:A:244:LEU:HD12	1.88	0.55
3:A:264:ALA:HB1	3:A:306:PHE:CD1	2.41	0.55
4:B:40:LEU:HD12	4:B:60:VAL:HG23	1.88	0.55
3:A:124:MET:HG2	3:A:183:VAL:HG12	1.88	0.55
3:A:248:ARG:NH2	3:A:287:GLN:HE21	2.05	0.55
3:A:237:ARG:NH2	3:A:238:LYS:HE2	2.23	0.54
3:A:271:GLN:NE2	3:A:316:LEU:CD1	2.70	0.54
3:A:296:ALA:HB3	3:A:297:PRO:HD3	1.89	0.54
4:B:160:ILE:HD12	4:B:160:ILE:O	2.07	0.54
4:B:155:MET:HG3	4:B:162:LEU:CD1	2.38	0.53
3:A:275:GLY:HA2	3:A:285:ILE:HD11	1.91	0.53
3:A:134:LYS:HB3	3:A:171:GLU:HG3	1.90	0.53
4:B:67:PRO:HD3	4:B:92:MET:CE	2.39	0.53
4:B:39:ASP:OD2	4:B:42:ALA:HB2	2.09	0.53
2:D:106:DC:H2'	2:D:107:DT:H71	1.91	0.53
3:A:221:ASN:HB3	3:A:277:ILE:HD12	1.90	0.53
4:B:158:PRO:HG2	4:B:160:ILE:HG13	1.91	0.52
3:A:175:ARG:NH1	3:A:175:ARG:HB3	2.25	0.52
4:B:127:PRO:HG2	4:B:197:LYS:HB2	1.92	0.52
4:B:67:PRO:CG	4:B:93:ALA:HB2	2.39	0.52
4:B:157:VAL:O	4:B:157:VAL:HG23	2.10	0.51
4:B:102:GLN:HG3	4:B:108:ALA:CB	2.32	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:119:VAL:HG22	4:B:173:THR:HG22	1.93	0.51
3:A:144:GLN:C	3:A:146:TYR:H	2.14	0.51
3:A:305:LYS:H	3:A:305:LYS:CD	2.23	0.51
2:D:107:DT:H4'	4:B:57:PHE:HB2	1.94	0.50
3:A:194:CYS:HA	3:A:197:LEU:HD12	1.92	0.50
3:A:135:VAL:O	3:A:139:ASN:ND2	2.45	0.50
3:A:305:LYS:H	3:A:305:LYS:HD2	1.77	0.50
3:A:265:SER:O	3:A:307:ASP:HB3	2.12	0.50
3:A:175:ARG:CZ	3:A:175:ARG:HB3	2.41	0.50
4:B:36:CYS:HB3	4:B:107:PRO:HB2	1.94	0.50
3:A:134:LYS:HD3	3:A:168:CYS:SG	2.52	0.50
4:B:12:VAL:O	4:B:13:ASP:CB	2.59	0.50
3:A:245:VAL:HB	3:A:248:ARG:CG	2.41	0.50
4:B:129:ARG:HG2	4:B:129:ARG:NH1	2.27	0.50
3:A:238:LYS:HB3	3:A:299:LEU:HD23	1.94	0.50
3:A:270:THR:HG1	3:A:273:GLU:HG3	1.77	0.49
4:B:67:PRO:HD3	4:B:92:MET:HE2	1.94	0.49
3:A:149:LYS:CG	3:A:150:SER:H	2.25	0.49
3:A:271:GLN:NE2	3:A:316:LEU:HD11	2.28	0.49
3:A:270:THR:O	3:A:274:ILE:HG13	2.13	0.49
3:A:264:ALA:O	3:A:306:PHE:HA	2.13	0.49
4:B:118:ILE:N	4:B:175:ALA:O	2.45	0.49
4:B:118:ILE:HB	4:B:175:ALA:HB3	1.96	0.48
3:A:305:LYS:O	3:A:306:PHE:CB	2.60	0.48
4:B:126:PHE:CZ	4:B:193:SER:HA	2.49	0.48
2:D:114:DG:H5''	3:A:247:GLY:O	2.13	0.48
2:D:104:DC:H2'	2:D:105:DC:C6	2.48	0.47
4:B:178:ARG:CB	4:B:178:ARG:HH11	2.26	0.47
3:A:162:ALA:O	3:A:165:TYR:HB3	2.14	0.47
3:A:164:LEU:O	3:A:164:LEU:HG	2.13	0.47
3:A:169:ARG:HG2	3:A:174:PRO:CB	2.43	0.47
3:A:223:CYS:HB2	3:A:269:ARG:HH21	1.78	0.47
1:C:15:DT:C5	2:D:101:DC:N4	2.82	0.47
4:B:17:HIS:CE1	4:B:22:VAL:HG13	2.49	0.47
1:C:15:DT:H3	2:D:102:DA:N6	2.12	0.47
4:B:155:MET:HB2	4:B:160:ILE:CD1	2.43	0.47
3:A:264:ALA:HB2	3:A:313:LEU:HD21	1.97	0.47
4:B:42:ALA:O	4:B:44:ALA:N	2.47	0.47
3:A:286:ARG:HH11	3:A:316:LEU:HD22	1.78	0.47
3:A:149:LYS:HG3	3:A:150:SER:H	1.79	0.47
1:C:4:DT:OP1	3:A:189:LYS:HD2	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:160:ILE:CG1	4:B:184:ALA:HB2	2.42	0.46
3:A:305:LYS:O	3:A:306:PHE:CD2	2.68	0.46
3:A:259:TYR:CE1	3:A:271:GLN:HG3	2.49	0.46
4:B:42:ALA:O	4:B:45:LEU:N	2.48	0.46
3:A:130:LEU:HD22	3:A:134:LYS:CD	2.43	0.46
3:A:211:THR:CG2	3:A:236:ALA:HB1	2.45	0.46
3:A:271:GLN:NE2	3:A:316:LEU:HD13	2.30	0.46
3:A:301:PRO:HD2	3:A:304:PHE:HB2	1.99	0.45
4:B:122:CYS:HB3	4:B:170:ILE:HB	1.97	0.45
3:A:134:LYS:HE3	3:A:168:CYS:HA	1.98	0.45
1:C:16:DG:H4'	3:A:153:GLY:O	2.16	0.45
4:B:32:VAL:HG21	4:B:110:PHE:CE1	2.51	0.45
2:D:110:DT:H4'	4:B:26:GLN:O	2.16	0.45
4:B:26:GLN:NE2	4:B:121:SER:OG	2.49	0.45
4:B:155:MET:HE1	4:B:157:VAL:O	2.16	0.45
2:D:103:DG:H2''	2:D:104:DC:O5'	2.17	0.45
3:A:282:ASP:OD1	3:A:282:ASP:N	2.50	0.45
3:A:272:LYS:O	3:A:276:ASP:HB2	2.16	0.45
3:A:283:VAL:O	3:A:286:ARG:HB3	2.17	0.45
4:B:50:ALA:HB1	4:B:60:VAL:HG13	1.98	0.45
4:B:95:ARG:HB3	4:B:99:ARG:CZ	2.47	0.45
4:B:191:VAL:O	4:B:195:PHE:HD1	2.00	0.45
3:A:175:ARG:HA	3:A:217:ARG:HH21	1.80	0.44
3:A:271:GLN:HE22	3:A:316:LEU:HD13	1.83	0.44
3:A:226:LYS:HD2	3:A:226:LYS:C	2.37	0.44
3:A:166:ILE:HD12	3:A:170:GLN:HG3	1.99	0.44
3:A:266:ALA:O	3:A:268:LYS:N	2.51	0.44
3:A:125:ALA:HB1	3:A:135:VAL:CG2	2.47	0.44
2:D:110:DT:H2'	2:D:111:DA:C8	2.52	0.44
3:A:157:ASP:HA	3:A:160:ALA:HB3	2.00	0.44
1:C:15:DT:C4	2:D:101:DC:N4	2.86	0.43
3:A:293:TYR:HB3	3:A:294:PRO:HD3	1.99	0.43
3:A:143:ARG:O	3:A:147:GLU:HG2	2.18	0.43
3:A:245:VAL:O	3:A:248:ARG:HG2	2.18	0.43
2:D:104:DC:H2'	2:D:105:DC:O4'	2.19	0.43
3:A:226:LYS:NZ	3:A:227:GLN:NE2	2.67	0.43
3:A:244:LEU:HD21	3:A:295:ARG:HG3	2.01	0.43
3:A:125:ALA:CB	3:A:135:VAL:HG22	2.48	0.43
3:A:245:VAL:HB	3:A:248:ARG:HG2	2.00	0.43
1:C:6:DT:H4'	4:B:161:VAL:HG11	2.00	0.43
3:A:136:ASP:HA	3:A:139:ASN:HD22	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:269:ARG:HH11	3:A:269:ARG:HG2	1.84	0.42
3:A:156:ASN:HD22	3:A:156:ASN:N	2.17	0.42
4:B:49:ASN:ND2	4:B:62:MET:HG2	2.33	0.42
4:B:95:ARG:HE	4:B:99:ARG:HH22	1.66	0.42
3:A:259:TYR:HB2	3:A:274:ILE:HD12	2.01	0.42
3:A:186:ILE:HG22	3:A:191:ILE:HG13	2.00	0.42
4:B:137:HIS:O	4:B:141:SER:OG	2.36	0.42
3:A:181:CYS:C	3:A:183:VAL:H	2.22	0.42
4:B:71:ALA:HA	4:B:80:VAL:O	2.19	0.42
4:B:73:ILE:HG12	4:B:79:MET:HE3	2.01	0.42
4:B:66:GLU:HA	4:B:67:PRO:HA	1.80	0.42
3:A:215:MET:SD	3:A:258:ILE:HD11	2.60	0.42
3:A:168:CYS:HB3	3:A:173:VAL:O	2.19	0.42
4:B:95:ARG:O	4:B:99:ARG:HD3	2.19	0.42
4:B:106:PHE:HA	4:B:107:PRO:HD3	1.73	0.42
3:A:157:ASP:OD2	3:A:186:ILE:HD13	2.19	0.42
4:B:96:LYS:O	4:B:100:ILE:HG13	2.19	0.42
1:C:9:DA:H2'	1:C:10:DA:C8	2.54	0.42
3:A:142:PHE:HE2	3:A:156:ASN:O	2.02	0.42
3:A:235:ILE:HG21	3:A:260:MET:CE	2.49	0.42
3:A:184:SER:O	3:A:185:ARG:HB3	2.20	0.42
3:A:164:LEU:CG	3:A:164:LEU:O	2.68	0.42
3:A:186:ILE:HG23	3:A:190:GLU:HB2	2.01	0.42
3:A:131:PRO:O	3:A:135:VAL:HG23	2.20	0.42
2:D:110:DT:O2	4:B:119:VAL:HG11	2.20	0.42
4:B:38:LEU:HD11	4:B:101:VAL:HG11	2.01	0.42
2:D:106:DC:H2''	2:D:107:DT:O5'	2.19	0.41
3:A:170:GLN:HG2	3:A:206:VAL:HG12	2.01	0.41
4:B:87:GLU:O	4:B:88:ASP:C	2.58	0.41
3:A:175:ARG:HA	3:A:217:ARG:HH22	1.81	0.41
3:A:209:ILE:HG23	3:A:214:PHE:CZ	2.55	0.41
3:A:221:ASN:HB2	3:A:277:ILE:HG21	2.01	0.41
2:D:112:DT:H1'	4:B:165:PHE:CZ	2.56	0.41
2:D:103:DG:H2''	2:D:104:DC:O4'	2.20	0.41
3:A:264:ALA:HB1	3:A:306:PHE:HE1	1.83	0.41
1:C:16:DG:O5'	1:C:16:DG:H2'	2.20	0.41
4:B:134:ALA:HB2	4:B:151:LEU:CD2	2.51	0.41
3:A:268:LYS:O	3:A:269:ARG:HD3	2.21	0.40
4:B:32:VAL:HG21	4:B:110:PHE:CD1	2.56	0.40
4:B:17:HIS:NE2	4:B:22:VAL:HG13	2.36	0.40
4:B:124:VAL:HG13	4:B:189:TYR:CE1	2.57	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:144:GLN:HA	3:A:147:GLU:HG2	2.04	0.40
3:A:163:CYS:C	3:A:165:TYR:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	202/204 (99%)	165 (82%)	25 (12%)	12 (6%)	2	3
4	B	185/200 (92%)	153 (83%)	25 (14%)	7 (4%)	4	9
All	All	387/404 (96%)	318 (82%)	50 (13%)	19 (5%)	3	5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	152	LYS
3	A	185	ARG
3	A	267	GLU
3	A	302	THR
3	A	305	LYS
3	A	306	PHE
4	B	13	ASP
3	A	149	LYS
3	A	183	VAL
3	A	208	LEU
4	B	43	ILE
4	B	68	LYS
3	A	133	ASN
3	A	209	ILE
3	A	246	PRO
4	B	51	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	B	66	GLU
4	B	156	LYS
4	B	107	PRO

### 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	
3	A	172/172 (100%)	149 (87%)	23 (13%)	5	11
4	B	160/171 (94%)	146 (91%)	14 (9%)	12	28
All	All	332/343 (97%)	295 (89%)	37 (11%)	8	17

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	123	THR
3	A	128	ILE
3	A	138	THR
3	A	143	ARG
3	A	147	GLU
3	A	149	LYS
3	A	150	SER
3	A	166	ILE
3	A	175	ARG
3	A	204	THR
3	A	208	LEU
3	A	211	THR
3	A	213	ASP
3	A	226	LYS
3	A	230	MET
3	A	238	LYS
3	A	260	MET
3	A	272	LYS
3	A	276	ASP
3	A	280	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	A	282	ASP
3	A	287	GLN
3	A	305	LYS
4	B	24	THR
4	B	35	ASP
4	B	48	ARG
4	B	53	ASN
4	B	65	ARG
4	B	66	GLU
4	B	102	GLN
4	B	129	ARG
4	B	141	SER
4	B	151	LEU
4	B	155	MET
4	B	156	LYS
4	B	178	ARG
4	B	179	ASP

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	116	ASN
3	A	129	ASN
3	A	139	ASN
3	A	156	ASN
3	A	227	GLN
3	A	271	GLN
3	A	287	GLN
4	B	17	HIS
4	B	102	GLN
4	B	187	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 carbohydrates 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.