



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:47 PM UTC

PDB ID : 1VOL / pdb_00001vol
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

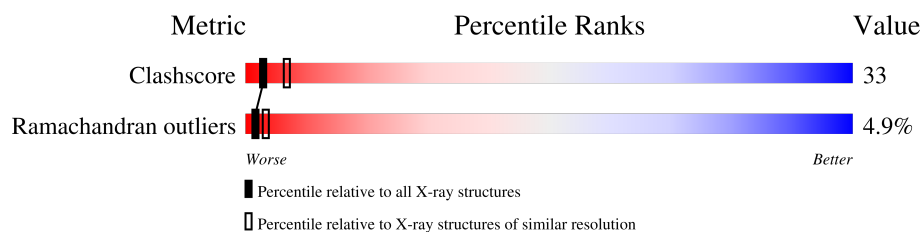
1 Overall quality at a glance

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	16	38% 56% 6%
2	D	16	12% 56% 31%
3	A	204	35% 57% 7% .
4	B	200	44% 40% 10% 6%

2 Entry composition [i](#)

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, 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. 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. 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')

Chain C: 



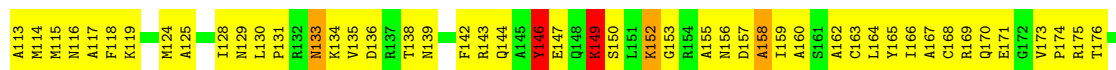
- Molecule 2: DNA (5'-D(*CP*AP*GP*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*C)-3')

Chain D: 

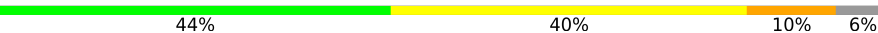


- Molecule 3: PROTEIN (TRANSCRIPTION FACTOR IIB (TFIIB))

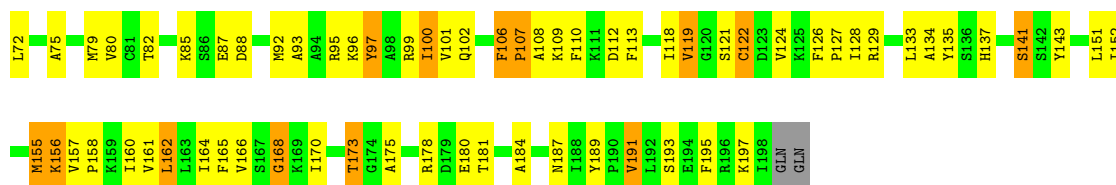
Chain A: 



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

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.90Å 78.00Å 134.70Å 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 ²)	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	0.79	0/374	1.35	3/577 (0.5%)
2	D	0.84	0/354	1.57	6/543 (1.1%)
3	A	0.84	0/1614	1.30	17/2175 (0.8%)
4	B	0.89	1/1505 (0.1%)	1.30	21/2026 (1.0%)
All	All	0.85	1/3847 (0.0%)	1.34	47/5321 (0.9%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	155	MET	SD-CE	-6.35	1.63	1.79

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	191	VAL	N-CA-C	-10.71	101.48	111.45
3	A	184	SER	N-CA-C	10.07	125.61	112.12
3	A	158	ALA	N-CA-C	-9.92	100.72	113.12
3	A	245	VAL	CA-C-N	8.20	130.08	119.84
3	A	245	VAL	C-N-CA	8.20	130.08	119.84
4	B	112	ASP	N-CA-C	7.96	124.62	113.56
3	A	207	ASP	N-CA-C	7.74	122.86	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	PHE	CA-C-N	7.62	127.51	119.05
3	A	300	PHE	C-N-CA	7.62	127.51	119.05
3	A	146	TYR	N-CA-C	-7.18	103.63	113.18
4	B	180	GLU	N-CA-C	-7.10	103.47	111.07
3	A	188	LYS	N-CA-C	-6.66	104.02	111.28
3	A	232	ALA	N-CA-C	-6.61	104.00	111.07
2	D	109	DT	C4'-C3'-O3'	-6.58	100.14	110.00
1	C	5	DA	C5'-C4'-C3'	-6.57	105.04	114.90
4	B	106	PHE	CA-C-N	6.41	127.86	119.84
4	B	106	PHE	C-N-CA	6.41	127.86	119.84
2	D	115	DC	O4'-C1'-C2'	-6.34	96.88	106.40
3	A	239	ALA	N-CA-C	-6.28	104.35	111.07
3	A	129	ASN	N-CA-C	6.21	120.15	112.58
2	D	108	DT	C5'-C4'-C3'	-6.10	105.75	114.90
4	B	100	ILE	N-CA-C	-6.07	105.22	110.74
4	B	72	LEU	N-CA-C	-5.96	98.69	108.41
4	B	155	MET	N-CA-C	5.95	118.86	110.23
4	B	49	ASN	N-CA-C	-5.83	105.83	113.17
4	B	162	LEU	N-CA-C	-5.81	101.60	110.14
3	A	152	LYS	N-CA-C	5.77	123.09	110.80
4	B	57	PHE	N-CA-C	5.68	117.66	108.41
2	D	109	DT	C5'-C4'-C3'	-5.67	106.39	114.90
3	A	208	LEU	N-CA-C	5.65	122.83	110.80
4	B	122	CYS	N-CA-CB	-5.54	102.92	111.46
3	A	149	LYS	N-CA-C	5.53	122.57	110.80
3	A	159	ILE	N-CA-C	-5.49	105.02	110.62
4	B	45	LEU	N-CA-C	5.44	118.72	111.75
4	B	164	ILE	CB-CA-C	-5.42	103.80	111.28
4	B	128	ILE	N-CA-C	5.35	116.44	108.46
1	C	10	DA	C5'-C4'-C3'	-5.31	106.94	114.90
4	B	119	VAL	N-CA-C	-5.20	100.96	108.71
2	D	101	DC	O4'-C1'-N1	5.16	116.14	108.40
3	A	266	ALA	N-CA-C	-5.14	99.86	110.80
4	B	152	ILE	CB-CA-C	-5.13	106.36	111.80
4	B	12	VAL	N-CA-C	5.13	125.36	111.00
4	B	168	GLY	N-CA-C	-5.12	107.47	114.64
4	B	173	THR	CB-CA-C	-5.11	101.61	110.45
4	B	141	SER	N-CA-C	5.08	117.86	109.72
2	D	104	DC	C5'-C4'-C3'	-5.08	107.28	114.90
1	C	13	DG	C5'-C4'-C3'	-5.03	107.36	114.90

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	132	0
4	B	1475	0	1558	88	0
All	All	3715	0	3568	236	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 33.

All (236) 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
4:B:79:MET:HE1	4:B:97:TYR:HB3	1.60	0.81
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:110:DT:O2	4:B:119:VAL:HG21	1.89	0.73
4:B:67:PRO:HG2	4:B:93:ALA:HB2	1.70	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
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: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
4:B:12:VAL:O	4:B:13:ASP:HB2	1.92	0.68
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:HG3	3:A:143:ARG:HH11	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
4:B:67:PRO:HD3	4:B:92:MET:HE3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:194:CYS:O	3:A:198:ILE:HG13	2.03	0.57
4:B:50:ALA:HA	4:B:62:MET:HA	1.86	0.57
3:A:115:MET:HB3	3:A:119:LYS:HZ3	1.69	0.57
4:B:54:PRO:HG2	4:B:55:LYS:HE2	1.87	0.57
2:D:104:DC:H2'	2:D:105:DC:H6	1.68	0.57
4:B:35:ASP:HB2	4:B:109:LYS:HB2	1.87	0.57
4:B:40:LEU:CD2	4:B:75:ALA:HB2	2.34	0.56
3:A:235:ILE:HG21	3:A:260:MET:HE3	1.86	0.56
3:A:149:LYS:HB2	3:A:149:LYS:NZ	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:HG2	4:B:129:ARG:HH11	1.71	0.56
4:B:155:MET:HE1	4:B:187:ASN:HD22	1.69	0.56
3:A:262:SER:OG	3:A:268:LYS:HA	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:144:GLN:C	3:A:146:TYR:H	2.14	0.55
3:A:264:ALA:HB1	3:A:306:PHE:CD1	2.41	0.55
3:A:124:MET:HG2	3:A:183:VAL:HG12	1.88	0.55
4:B:40:LEU:HD12	4:B:60:VAL:HG23	1.88	0.55
3:A:114:MET:HE2	3:A:115:MET:HE2	1.89	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
3:A:305:LYS:O	3:A:306:PHE:HB2	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:67:PRO:HD3	4:B:92:MET:CE	2.39	0.52
4:B:158:PRO:HG2	4:B:160:ILE:HG13	1.91	0.52
3:A:175:ARG:HB3	3:A:175:ARG:NH1	2.25	0.52
4:B:67:PRO:CG	4:B:93:ALA:HB2	2.39	0.52
4:B:127:PRO:HG2	4:B:197:LYS:HB2	1.92	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
4:B:119:VAL:HG22	4:B:173:THR:HG22	1.93	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:HB3	3:A:175:ARG:CZ	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
3:A:238:LYS:HB3	3:A:299:LEU:HD23	1.94	0.50
3:A:245:VAL:HB	3:A:248:ARG:CG	2.41	0.50
4:B:12:VAL:O	4:B:13:ASP:CB	2.59	0.50
4:B:129:ARG:HG2	4:B:129:ARG:NH1	2.27	0.50
3:A:149:LYS:CG	3:A:150:SER:H	2.25	0.49
3:A:226:LYS:HD2	3:A:226:LYS:C	2.37	0.49
3:A:271:GLN:NE2	3:A:316:LEU:HD11	2.28	0.49
3:A:264:ALA:O	3:A:306:PHE:HA	2.13	0.49
3:A:270:THR:O	3:A:274:ILE:HG13	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
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
4:B:178:ARG:CB	4:B:178:ARG:HH11	2.26	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
3:A:264:ALA:HB2	3:A:313:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:42:ALA:O	4:B:44:ALA:N	2.47	0.47
4:B:155:MET:HB2	4:B:160:ILE:CD1	2.43	0.47
3:A:149:LYS:HG3	3:A:150:SER:H	1.79	0.47
3:A:181:CYS:C	3:A:183:VAL:H	2.22	0.47
3:A:286:ARG:HH11	3:A:316:LEU:HD22	1.78	0.47
1:C:4:DT:OP1	3:A:189:LYS:HD2	2.15	0.47
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
4:B:87:GLU:O	4:B:88:ASP:C	2.58	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
1:C:16:DG:H4'	3:A:153:GLY:O	2.16	0.45
3:A:134:LYS:HE3	3:A:168:CYS:HA	1.98	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
2:D:103:DG:H2''	2:D:104:DC:O5'	2.17	0.45
3:A:163:CYS:C	3:A:165:TYR:H	2.25	0.45
3:A:282:ASP:N	3:A:282:ASP:OD1	2.50	0.45
3:A:272:LYS:O	3:A:276:ASP:HB2	2.16	0.45
3:A:270:THR:HG1	3:A:273:GLU:HG3	1.78	0.45
3:A:283:VAL:O	3:A:286:ARG:HB3	2.17	0.45
4:B:16:LYS:C	4:B:18:PRO:HD3	2.42	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:167:ALA:O	3:A:168:CYS:C	2.60	0.44
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: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
2:D:110:DT:H2'	2:D:111:DA:C8	2.52	0.44
3:A:125:ALA:HB1	3:A:135:VAL:CG2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:133:LEU:HD23	4:B:133:LEU:C	2.43	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
4:B:113:PHE:CD1	4:B:113:PHE:C	2.97	0.43
1:C:6:DT:H4'	4:B:161:VAL:HG11	2.00	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
3:A:136:ASP:HA	3:A:139:ASN:HD22	1.83	0.43
3:A:156:ASN:N	3:A:156:ASN:HD22	2.17	0.42
3:A:269:ARG:HH11	3:A:269:ARG:HG2	1.84	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:186:ILE:HG22	3:A:191:ILE:HG13	2.00	0.42
3:A:259:TYR:HB2	3:A:274:ILE:HD12	2.01	0.42
4:B:137:HIS:O	4:B:141:SER:OG	2.36	0.42
4:B:71:ALA:HA	4:B:80:VAL:O	2.19	0.42
4:B:155:MET:HE2	4:B:155:MET:HB3	1.44	0.42
3:A:310:VAL:C	3:A:312:LYS:N	2.76	0.42
3:A:215:MET:SD	3:A:258:ILE:HD11	2.60	0.42
4:B:66:GLU:HA	4:B:67:PRO:HA	1.80	0.42
3:A:157:ASP:OD2	3:A:186:ILE:HD13	2.19	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:96:LYS:O	4:B:100:ILE:HG13	2.19	0.42
4:B:106:PHE:HA	4:B:107:PRO:HD3	1.73	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:184:SER:O	3:A:185:ARG:HB3	2.20	0.42
3:A:164:LEU:O	3:A:164:LEU:CG	2.68	0.42
3:A:186:ILE:HG23	3:A:190:GLU:HB2	2.01	0.42
3:A:217:ARG:O	3:A:218:PHE:C	2.63	0.42
2:D:110:DT:O2	4:B:119:VAL:HG11	2.20	0.42
3:A:131:PRO:O	3:A:135:VAL:HG23	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
3:A:310:VAL:C	3:A:312:LYS:H	2.28	0.41
2:D:112:DT:H1'	4:B:165:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:A:235:ILE:HG21	3:A:260:MET:CE	2.49	0.41
4:B:46:GLN:O	4:B:47:ALA:C	2.64	0.41
1:C:16:DG:H2'	1:C:16:DG:O5'	2.20	0.41
3:A:124:MET:O	3:A:125:ALA:C	2.64	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
3:A:114:MET:HE3	3:A:118:PHE:CE2	2.57	0.40
4:B:32:VAL:HG21	4:B:110:PHE:CD1	2.56	0.40
4:B:160:ILE:HD12	4:B:160:ILE:C	2.47	0.40
3:A:144:GLN:HA	3:A:147:GLU:HG2	2.04	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

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%)	1	2
4	B	185/200 (92%)	153 (83%)	25 (14%)	7 (4%)	2	5
All	All	387/404 (96%)	318 (82%)	50 (13%)	19 (5%)	1	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	152	LYS

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

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.