



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 1NFK / pdb_00001nfk
Title : STRUCTURE OF THE NUCLEAR FACTOR KAPPA-B (NF-KB) P50 HO-MODIMER
Authors : Ghosh, G.; Van Duyne, G.; Ghosh, S.; Sigler, P.B.
Deposited on : 1995-02-28
Resolution : 2.30 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

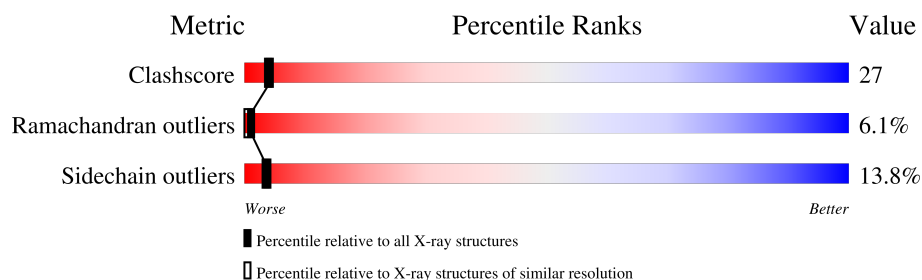
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	11	36% 45% 18%
1	D	11	55% 36% 9%
2	A	325	51% 34% 9% • •
2	B	325	38% 43% 13% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7477 atoms, of which 1810 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(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	11	Total	C	H	N	O	P	0	0	0
			246	107	24	40	65	10			
1	D	11	Total	C	H	N	O	P	0	0	0
			246	107	24	40	65	10			

- Molecule 2 is a protein called PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	312	Total	C	H	N	O	S	0	0	0
			3017	1554	564	428	459	12			
2	B	312	Total	C	H	N	O	S	0	0	0
			3017	1554	564	428	459	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	25	Total	H	O	0	0
			75	50	25		
3	D	26	Total	H	O	0	0
			78	52	26		
3	A	152	Total	H	O	0	0
			456	304	152		
3	B	114	Total	H	O	0	0
			342	228	114		

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.

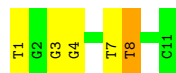
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3')

Chain C: 



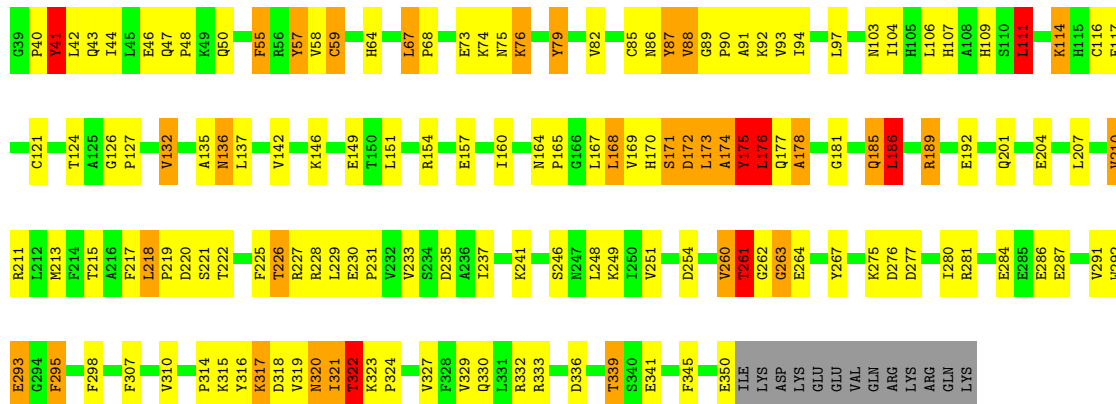
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3')

Chain D: 



- Molecule 2: PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB))

Chain A: 



- Molecule 2: PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB))

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.20Å 132.10Å 80.10Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.340	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7477	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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	1.54	1/248 (0.4%)	1.49	2/381 (0.5%)
1	D	1.74	2/248 (0.8%)	1.51	1/381 (0.3%)
2	A	0.74	0/2505	1.22	24/3384 (0.7%)
2	B	0.66	0/2505	1.16	27/3384 (0.8%)
All	All	0.83	3/5506 (0.1%)	1.23	54/7530 (0.7%)

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
2	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	DT	O3'-P	-6.81	1.50	1.61
1	D	7	DT	C5'-C4'	-6.60	1.39	1.52
1	C	8	DT	C5'-C4'	-5.68	1.40	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	GLU	N-CA-C	9.52	124.89	113.28
2	A	173	LEU	N-CA-C	8.11	121.40	109.07
2	A	126	GLY	CA-C-N	8.05	127.61	119.24
2	A	126	GLY	C-N-CA	8.05	127.61	119.24
2	A	261	THR	N-CA-C	-7.67	94.47	110.80
2	A	41	TYR	N-CA-C	7.19	118.66	108.74
2	B	100	ASN	N-CA-C	-7.12	96.95	108.41
2	A	260	VAL	N-CA-C	-7.07	99.44	109.63
2	A	218	LEU	CA-C-N	7.06	128.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	LEU	C-N-CA	7.06	128.66	119.84
2	A	185	GLN	N-CA-C	7.02	120.56	110.24
2	A	320	ASN	N-CA-C	6.99	125.69	110.80
2	A	254	ASP	N-CA-C	6.80	119.53	111.71
1	C	9	DC	C5'-C4'-C3'	-6.76	104.75	114.90
2	B	205	MET	N-CA-C	6.76	125.21	110.80
2	B	42	LEU	N-CA-C	-6.74	98.71	109.76
2	B	341	GLU	N-CA-C	-6.22	100.35	109.50
2	A	186	LEU	N-CA-C	6.21	118.93	110.55
1	C	8	DT	C4-C5-C7	-6.16	113.16	122.40
2	B	272	LYS	N-CA-C	6.14	119.27	110.24
2	B	99	THR	N-CA-C	6.10	119.46	109.76
2	B	271	ASP	N-CA-C	-5.79	102.19	110.59
2	B	147	VAL	N-CA-C	5.77	116.55	110.72
2	B	230	GLU	CA-C-N	5.76	125.52	119.76
2	B	230	GLU	C-N-CA	5.76	125.52	119.76
2	A	57	TYR	N-CA-C	-5.71	102.07	110.52
2	A	168	LEU	N-CA-C	5.64	119.34	112.23
2	A	111	LEU	N-CA-C	-5.63	100.81	109.76
2	A	339	THR	N-CA-C	5.62	118.23	109.52
2	A	295	PHE	N-CA-C	5.47	117.82	108.90
2	A	55	PHE	N-CA-C	-5.40	102.29	110.28
2	A	67	LEU	CA-C-N	5.36	125.83	120.52
2	A	67	LEU	C-N-CA	5.36	125.83	120.52
2	A	59	CYS	N-CA-C	5.34	117.85	111.71
1	D	8	DT	C5'-C4'-C3'	-5.27	107.00	114.90
2	B	110	SER	N-CA-C	5.25	117.63	108.76
2	B	90	PRO	N-CA-C	-5.22	103.00	111.14
2	A	50	GLN	N-CA-C	5.20	117.74	111.40
2	B	187	THR	N-CA-C	5.18	118.14	109.96
2	B	348	TYR	CA-C-N	5.18	126.31	119.84
2	B	348	TYR	C-N-CA	5.18	126.31	119.84
2	B	218	LEU	CA-C-N	5.16	126.29	119.84
2	B	218	LEU	C-N-CA	5.16	126.29	119.84
2	B	229	LEU	N-CA-C	-5.16	100.89	108.99
2	B	311	PHE	N-CA-C	5.14	116.47	109.18
2	A	263	GLY	N-CA-C	-5.11	101.06	113.18
2	B	98	VAL	N-CA-C	5.08	115.01	108.82
2	B	265	GLU	N-CA-C	5.06	117.80	109.76
2	B	343	LYS	CA-C-N	5.05	124.81	119.76
2	B	343	LYS	C-N-CA	5.05	124.81	119.76
2	A	146	LYS	N-CA-C	5.01	118.97	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	253	MET	CA-C-N	5.01	127.26	120.65
2	B	253	MET	C-N-CA	5.01	127.26	120.65
2	B	44	ILE	CB-CA-C	-5.00	105.90	111.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	175	TYR	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	222	24	125	5	0
1	D	222	24	126	7	0
2	A	2453	564	2449	123	0
2	B	2453	564	2451	158	0
3	A	152	304	0	10	0
3	B	114	228	0	4	0
3	C	25	50	0	1	0
3	D	26	52	0	2	0
All	All	5667	1810	5151	283	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 27.

All (283) 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:C:9:DC:H2'	2:A:59:CYS:SG	1.97	1.05
1:C:1:DT:H2''	1:C:2:DG:H5'	1.42	0.99
2:B:218:LEU:HB2	2:B:227:ARG:HB3	1.41	0.99
2:A:92:LYS:HG2	2:A:124:THR:HG22	1.44	0.98
2:B:147:VAL:HG12	2:B:202:THR:HG22	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:88:VAL:HB	2:A:218:LEU:HD13	1.53	0.88
2:B:83:LYS:HE3	2:B:85:CYS:SG	2.15	0.85
2:A:90:PRO:HG3	2:A:127:PRO:HA	1.58	0.85
2:B:281:ARG:HG3	2:B:295:PHE:CE1	2.13	0.84
2:A:286:GLU:HG2	2:A:291:VAL:HA	1.59	0.82
2:A:46:GLU:HG2	2:A:79:TYR:O	1.79	0.81
2:B:255:ARG:NH1	2:B:264:GLU:HB3	1.96	0.80
2:A:261:THR:O	2:A:315:LYS:HA	1.82	0.80
2:B:94:ILE:HG22	2:B:122:THR:HG22	1.65	0.79
2:B:59:CYS:SG	2:B:60:GLU:HG3	2.23	0.77
2:B:218:LEU:HD11	2:B:229:LEU:HD22	1.68	0.76
2:B:260:VAL:HG23	2:B:348:TYR:O	1.86	0.75
2:B:255:ARG:HH11	2:B:264:GLU:HB3	1.51	0.74
2:B:95:VAL:HG23	2:B:121:CYS:HB2	1.69	0.74
2:A:58:VAL:HG23	3:A:440:HOH:O	1.87	0.73
2:A:319:VAL:HG23	2:A:320:ASN:H	1.53	0.73
2:A:41:TYR:HD1	2:A:85:CYS:HB2	1.53	0.73
2:B:349:PRO:HG2	2:B:350:GLU:H	1.54	0.72
2:A:41:TYR:CD1	2:A:85:CYS:HB2	2.25	0.71
2:A:40:PRO:HA	2:A:86:ASN:HB2	1.72	0.71
2:B:107:HIS:HD2	2:B:109:HIS:H	1.39	0.71
2:A:173:LEU:HG	2:A:174:ALA:H	1.56	0.70
2:A:44:ILE:HA	2:A:82:VAL:HG12	1.73	0.70
2:B:50:GLN:HG3	2:B:236:ALA:O	1.92	0.70
2:A:225:PHE:O	2:A:226:THR:HG23	1.92	0.70
2:A:165:PRO:HB2	2:A:174:ALA:HB3	1.74	0.69
2:B:40:PRO:HA	2:B:86:ASN:HB3	1.73	0.69
2:A:220:ASP:HB2	2:A:226:THR:OG1	1.93	0.69
2:B:109:HIS:CD2	2:B:142:VAL:H	2.11	0.69
2:A:41:TYR:HE1	2:A:85:CYS:SG	2.16	0.69
1:C:3:DG:H1'	1:C:4:DG:H5''	1.75	0.69
2:B:46:GLU:HG2	2:B:79:TYR:O	1.94	0.67
2:B:91:ALA:HB3	2:B:125:ALA:HB3	1.75	0.67
2:B:286:GLU:HG2	2:B:291:VAL:HG21	1.76	0.67
2:B:254:ASP:HB2	2:B:267:TYR:H	1.59	0.66
1:C:1:DT:C2'	1:C:2:DG:H5'	2.23	0.66
2:A:165:PRO:CB	2:A:174:ALA:HB3	2.25	0.65
1:D:4:DG:P	2:B:305:ARG:HH12	2.19	0.65
2:A:218:LEU:HD21	2:A:229:LEU:HD11	1.79	0.65
2:A:160:ILE:HG22	2:A:186:LEU:HD13	1.79	0.65
2:A:218:LEU:HD11	2:A:229:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:HIS:HD2	2:B:142:VAL:HG22	1.61	0.65
2:B:228:ARG:HG2	2:B:229:LEU:H	1.62	0.65
2:A:310:VAL:HG11	2:B:252:ARG:NH1	2.12	0.64
2:B:42:LEU:HD23	2:B:216:ALA:HB2	1.77	0.64
2:B:88:VAL:HB	2:B:218:LEU:HG	1.79	0.64
2:B:155:MET:HE2	2:B:169:VAL:HG13	1.78	0.64
2:A:176:LEU:HB3	3:A:406:HOH:O	1.97	0.64
2:B:107:HIS:HE1	2:B:206:ASP:O	1.81	0.63
3:C:33:HOH:O	2:A:57:TYR:HB3	1.98	0.63
2:A:211:ARG:HD3	2:A:233:VAL:HG22	1.78	0.63
2:B:145:LYS:N	2:B:145:LYS:HD2	2.13	0.63
2:A:280:ILE:HD12	2:A:298:PHE:CE1	2.35	0.62
2:B:87:TYR:HE1	2:B:89:GLY:HA2	1.65	0.62
2:B:276:ASP:HB2	3:B:372:HOH:O	1.98	0.62
2:A:41:TYR:CE1	2:A:85:CYS:SG	2.92	0.62
2:B:283:TYR:OH	2:B:342:PRO:HB3	1.98	0.62
2:A:173:LEU:HG	2:A:174:ALA:N	2.15	0.62
2:A:215:THR:OG1	2:A:231:PRO:HB3	2.00	0.61
2:A:90:PRO:O	2:A:225:PHE:HE1	1.82	0.61
2:B:260:VAL:HG13	2:B:316:TYR:HB2	1.82	0.60
2:A:322:THR:HG22	2:A:323:LYS:H	1.66	0.60
2:A:88:VAL:CB	2:A:218:LEU:HD13	2.28	0.60
2:A:97:LEU:HG	2:A:111:LEU:HD22	1.83	0.60
2:B:49:LYS:HB2	2:B:68:PRO:HG2	1.83	0.59
2:B:160:ILE:HG22	2:B:160:ILE:O	2.03	0.59
2:A:281:ARG:HG3	2:A:295:PHE:CE1	2.37	0.59
2:A:284:GLU:O	2:A:291:VAL:HB	2.03	0.59
2:A:329:VAL:HG23	2:A:345:PHE:HB2	1.85	0.59
2:A:109:HIS:HD2	2:A:142:VAL:HG22	1.67	0.59
2:B:322:THR:O	2:B:323:LYS:HB3	2.03	0.58
2:A:135:ALA:O	2:A:136:ASN:HB2	2.04	0.57
2:A:321:ILE:HG12	2:A:322:THR:H	1.69	0.57
2:B:99:THR:HB	2:B:105:HIS:H	1.68	0.57
2:B:326:SER:HA	2:B:346:LEU:HD12	1.86	0.57
2:A:316:TYR:O	2:A:318:ASP:N	2.36	0.57
2:B:187:THR:H	2:B:190:GLU:HB3	1.70	0.57
2:A:175:TYR:HA	3:A:494:HOH:O	2.04	0.57
2:B:95:VAL:CG2	2:B:121:CYS:HB2	2.36	0.56
2:B:336:ASP:OD2	2:B:338:GLU:HB2	2.05	0.56
2:A:75:ASN:O	2:A:76:LYS:HG3	2.06	0.56
2:B:44:ILE:HG13	2:B:232:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLU:HB3	2:B:81:GLN:HB2	1.87	0.56
2:B:94:ILE:HA	2:B:121:CYS:O	2.05	0.56
2:A:67:LEU:HD12	2:A:68:PRO:HD2	1.87	0.56
2:B:93:VAL:O	2:B:122:THR:HA	2.04	0.56
2:A:40:PRO:HB2	2:A:88:VAL:HG21	1.88	0.56
2:B:54:ARG:HB2	2:B:240:SER:OG	2.06	0.56
2:B:93:VAL:HB	2:B:123:VAL:HG12	1.86	0.55
2:B:327:VAL:CG2	2:B:345:PHE:HB3	2.36	0.55
2:B:184:ARG:HD2	2:B:185:GLN:H	1.72	0.55
2:B:199:VAL:HG12	2:B:203:LYS:HE3	1.87	0.55
2:A:79:TYR:CD2	2:A:135:ALA:HB2	2.42	0.55
2:B:143:THR:HG22	2:B:145:LYS:H	1.71	0.54
2:A:109:HIS:HE1	2:A:207:LEU:O	1.90	0.54
2:B:176:LEU:HD22	2:B:184:ARG:HG2	1.89	0.54
2:B:316:TYR:C	2:B:318:ASP:H	2.13	0.54
2:B:141:HIS:HD2	2:B:142:VAL:O	1.91	0.54
2:B:265:GLU:HA	2:B:311:PHE:O	2.07	0.54
2:A:281:ARG:HE	2:A:293:GLU:HG3	1.73	0.54
2:A:174:ALA:O	2:A:175:TYR:C	2.51	0.53
2:A:284:GLU:HB2	2:A:327:VAL:HG12	1.90	0.53
2:A:93:VAL:HG21	2:A:132:VAL:HG21	1.91	0.53
2:A:164:ASN:N	2:A:165:PRO:HD3	2.23	0.53
1:D:3:DG:H1'	1:D:4:DG:H5'	1.89	0.53
2:B:107:HIS:CE1	2:B:206:ASP:O	2.61	0.53
2:B:281:ARG:NE	2:B:293:GLU:HG3	2.24	0.53
2:B:166:GLY:HA3	2:B:174:ALA:HA	1.90	0.53
2:B:135:ALA:O	2:B:136:ASN:ND2	2.42	0.52
2:A:321:ILE:HD13	2:A:321:ILE:N	2.24	0.52
2:B:153:ALA:O	2:B:157:GLU:HG2	2.08	0.52
2:A:329:VAL:CG2	2:A:345:PHE:HB2	2.40	0.52
2:B:90:PRO:O	2:B:225:PHE:HE1	1.93	0.52
2:B:79:TYR:N	2:B:79:TYR:CD1	2.78	0.52
2:B:113:GLY:O	2:B:116:CYS:HB2	2.08	0.52
2:B:41:TYR:O	2:B:84:ILE:HD12	2.10	0.52
2:B:148:PHE:HA	2:B:202:THR:HG21	1.91	0.52
2:A:175:TYR:O	2:A:176:LEU:HB2	2.10	0.51
2:A:73:GLU:OE2	2:A:74:LYS:HD2	2.11	0.51
2:A:275:LYS:HG3	2:A:276:ASP:N	2.25	0.51
2:A:217:PHE:HE1	2:A:228:ARG:HB2	1.75	0.51
2:A:276:ASP:HB2	3:A:468:HOH:O	2.09	0.51
2:B:105:HIS:HD2	2:B:168:LEU:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:HIS:HD2	2:A:109:HIS:H	1.59	0.51
2:B:184:ARG:HD2	3:B:475:HOH:O	2.10	0.51
2:A:106:LEU:HD13	2:A:154:ARG:HB3	1.92	0.51
2:B:186:LEU:HB2	2:B:191:LYS:HE3	1.91	0.51
2:A:317:LYS:O	2:A:320:ASN:ND2	2.44	0.51
1:D:4:DG:OP2	2:B:305:ARG:NH1	2.44	0.50
2:A:114:LYS:NZ	3:A:438:HOH:O	2.44	0.50
2:A:307:PHE:CD1	2:B:305:ARG:HG3	2.46	0.50
2:B:164:ASN:N	2:B:165:PRO:HD3	2.27	0.50
2:A:215:THR:HG1	2:A:231:PRO:HB3	1.76	0.50
3:D:28:HOH:O	2:B:57:TYR:HB3	2.10	0.50
2:B:186:LEU:HA	2:B:190:GLU:OE2	2.11	0.49
3:D:15:HOH:O	2:B:241:LYS:HD2	2.12	0.49
2:A:317:LYS:HB2	2:A:320:ASN:ND2	2.27	0.49
2:A:322:THR:HB	3:A:477:HOH:O	2.12	0.49
2:B:109:HIS:HE1	2:B:207:LEU:O	1.95	0.49
2:B:155:MET:HE3	2:B:201:GLN:NE2	2.27	0.49
2:B:218:LEU:HD23	2:B:227:ARG:HH21	1.77	0.49
2:B:282:PHE:HA	2:B:328:PHE:O	2.13	0.49
2:B:109:HIS:HB3	2:B:140:LEU:O	2.12	0.49
2:B:254:ASP:CB	2:B:267:TYR:H	2.25	0.49
2:B:268:LEU:O	2:B:308:ALA:HA	2.13	0.49
2:A:261:THR:HA	2:A:315:LYS:HE2	1.95	0.49
2:B:70:ALA:O	2:B:71:SER:HB3	2.13	0.49
2:A:228:ARG:NH2	3:A:486:HOH:O	2.46	0.49
2:B:42:LEU:HD13	2:B:43:GLN:N	2.28	0.49
2:B:299:SER:HB3	2:B:300:PRO:HD2	1.95	0.49
2:B:332:ARG:HB2	2:B:339:THR:HG22	1.93	0.48
2:A:109:HIS:CD2	2:A:142:VAL:H	2.31	0.48
2:B:218:LEU:HD13	2:B:227:ARG:O	2.12	0.48
2:A:42:LEU:O	2:A:43:GLN:NE2	2.46	0.48
2:A:260:VAL:O	2:A:261:THR:CB	2.62	0.48
2:A:321:ILE:HG12	2:A:322:THR:N	2.27	0.48
2:A:218:LEU:HB2	2:A:227:ARG:HB2	1.95	0.48
2:A:136:ASN:N	2:A:136:ASN:HD22	2.12	0.48
2:A:322:THR:CG2	2:A:323:LYS:H	2.24	0.48
2:B:116:CYS:SG	2:B:121:CYS:CB	3.02	0.48
2:B:87:TYR:CE1	2:B:89:GLY:HA2	2.47	0.48
2:B:109:HIS:CD2	2:B:142:VAL:HG22	2.46	0.48
2:A:189:ARG:NH1	3:A:445:HOH:O	2.47	0.48
2:B:160:ILE:HA	2:B:184:ARG:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:PHE:CE1	2:A:228:ARG:HB2	2.49	0.47
2:A:171:SER:O	2:A:172:ASP:HB3	2.14	0.47
2:A:350:GLU:H	2:A:350:GLU:HG2	1.47	0.47
2:A:281:ARG:HD3	2:A:330:GLN:OE1	2.14	0.47
2:B:46:GLU:OE2	2:B:78:SER:HB2	2.15	0.47
2:A:40:PRO:HG3	2:A:88:VAL:HG11	1.97	0.47
2:B:150:THR:O	2:B:154:ARG:HG2	2.14	0.47
2:B:199:VAL:O	2:B:203:LYS:HG3	2.15	0.47
1:D:8:DT:H5''	2:B:57:TYR:CE2	2.50	0.47
2:B:42:LEU:HB3	2:B:232:VAL:HG21	1.97	0.47
2:A:314:PRO:HA	3:A:428:HOH:O	2.15	0.46
2:B:100:ASN:HA	2:B:211:ARG:NE	2.29	0.46
2:B:211:ARG:HG2	2:B:236:ALA:HA	1.96	0.46
2:B:286:GLU:HG3	2:B:287:GLU:H	1.80	0.46
2:B:114:LYS:N	2:B:114:LYS:HE3	2.30	0.46
2:B:187:THR:N	2:B:190:GLU:HB3	2.30	0.46
2:A:47:GLN:OE1	2:A:48:PRO:HD2	2.14	0.46
2:A:91:ALA:HB1	2:A:217:PHE:O	2.16	0.46
2:B:98:VAL:HB	2:B:105:HIS:O	2.16	0.46
2:A:320:ASN:HA	2:A:321:ILE:HD13	1.98	0.46
2:B:83:LYS:HB3	2:B:83:LYS:HE2	1.76	0.46
2:B:101:GLY:C	2:B:103:ASN:H	2.24	0.46
2:A:116:CYS:HB2	3:A:482:HOH:O	2.16	0.46
2:B:254:ASP:HB3	2:B:266:ILE:HG23	1.97	0.46
2:B:144:LYS:HG3	2:B:207:LEU:CD2	2.46	0.46
2:B:292:TRP:HB2	3:B:471:HOH:O	2.16	0.46
2:A:218:LEU:O	2:A:227:ARG:HG3	2.16	0.45
2:A:104:ILE:HG13	2:A:104:ILE:O	2.16	0.45
2:B:47:GLN:OE1	2:B:48:PRO:HD2	2.16	0.45
2:B:262:GLY:H	2:B:315:LYS:HA	1.82	0.45
2:A:316:TYR:O	2:A:317:LYS:C	2.60	0.45
2:A:55:PHE:CD1	2:A:55:PHE:N	2.83	0.45
2:B:144:LYS:HE2	3:B:405:HOH:O	2.15	0.45
2:B:218:LEU:N	2:B:218:LEU:HD12	2.32	0.45
2:B:336:ASP:O	2:B:337:LEU:HB2	2.16	0.45
2:A:189:ARG:HA	2:A:189:ARG:HD3	1.62	0.45
2:B:318:ASP:OD1	2:B:321:ILE:HG12	2.17	0.45
2:A:94:ILE:O	2:A:94:ILE:HG13	2.17	0.45
2:B:42:LEU:HB3	2:B:232:VAL:CG2	2.47	0.45
2:B:326:SER:CA	2:B:346:LEU:HD12	2.47	0.45
2:A:261:THR:HG22	2:A:262:GLY:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ARG:O	2:B:193:ILE:HG12	2.16	0.45
2:A:116:CYS:SG	2:A:121:CYS:CB	3.04	0.44
2:A:171:SER:O	2:A:172:ASP:CB	2.65	0.44
2:A:177:GLN:O	2:A:178:ALA:HB3	2.16	0.44
2:B:82:VAL:HG22	2:B:132:VAL:HG23	1.98	0.44
2:B:88:VAL:CB	2:B:218:LEU:HG	2.46	0.44
2:A:267:TYR:OH	2:B:252:ARG:HB3	2.17	0.44
1:D:8:DT:OP1	2:B:143:THR:HG23	2.18	0.44
2:A:261:THR:HG22	2:A:262:GLY:H	1.83	0.44
2:B:184:ARG:NH2	2:B:187:THR:HG23	2.33	0.44
2:B:281:ARG:HD2	2:B:332:ARG:CZ	2.47	0.43
2:A:176:LEU:HD22	2:A:177:GLN:NE2	2.33	0.43
2:B:176:LEU:HD23	2:B:176:LEU:HA	1.80	0.43
2:A:293:GLU:OE2	2:A:295:PHE:CE2	2.72	0.43
2:B:212:LEU:HB2	2:B:234:SER:OG	2.18	0.43
2:A:40:PRO:CA	2:A:86:ASN:HB2	2.42	0.43
2:A:170:HIS:O	2:A:172:ASP:N	2.52	0.43
2:A:333:ARG:HB3	2:A:336:ASP:OD1	2.19	0.43
2:B:218:LEU:HD22	2:B:227:ARG:HE	1.84	0.43
2:B:318:ASP:C	2:B:319:VAL:HG12	2.43	0.43
2:B:176:LEU:O	2:B:177:GLN:HB3	2.18	0.43
2:A:211:ARG:HD3	2:A:233:VAL:CG2	2.46	0.43
2:B:76:LYS:O	2:B:76:LYS:HG2	2.19	0.43
2:A:67:LEU:HD21	2:A:237:ILE:HD13	1.99	0.43
2:B:146:LYS:O	2:B:150:THR:HG23	2.19	0.42
2:B:297:ASP:HB3	2:B:312:LYS:HB2	2.01	0.42
2:A:176:LEU:HD22	2:A:176:LEU:HA	1.67	0.42
2:A:246:SER:HB3	2:A:333:ARG:HH22	1.84	0.42
2:A:327:VAL:HG23	2:A:345:PHE:HB3	2.02	0.42
2:B:63:SER:O	2:B:64:HIS:HB3	2.19	0.42
2:B:322:THR:O	2:B:323:LYS:CB	2.67	0.42
2:B:41:TYR:O	2:B:84:ILE:HA	2.19	0.42
2:B:172:ASP:O	2:B:175:TYR:CE2	2.72	0.42
2:B:195:ARG:NH2	2:B:196:GLN:HG2	2.35	0.42
2:B:253:MET:HE2	2:B:266:ILE:HD13	2.02	0.42
2:B:263:GLY:C	2:B:312:LYS:HG3	2.44	0.42
1:D:1:DT:C2	2:A:64:HIS:O	2.73	0.42
2:B:90:PRO:HB2	2:B:225:PHE:HZ	1.84	0.42
2:B:229:LEU:HD12	2:B:229:LEU:HA	1.88	0.42
2:B:282:PHE:CD2	2:B:329:VAL:HG22	2.55	0.42
2:A:106:LEU:HD23	2:A:168:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:GLN:HA	2:A:204:GLU:CG	2.49	0.41
2:B:172:ASP:O	2:B:175:TYR:HE2	2.03	0.41
2:B:317:LYS:HG3	2:B:317:LYS:O	2.19	0.41
2:A:189:ARG:HG3	2:A:189:ARG:HH11	1.85	0.41
2:B:159:CYS:HB3	2:B:176:LEU:HD13	2.02	0.41
2:A:175:TYR:CD1	2:A:175:TYR:N	2.88	0.41
2:B:143:THR:CG2	2:B:145:LYS:HD3	2.51	0.41
2:B:44:ILE:HA	2:B:82:VAL:HG12	2.02	0.41
2:B:260:VAL:HG22	2:B:347:TYR:HB3	2.01	0.41
2:A:210:VAL:HG12	2:A:237:ILE:HB	2.03	0.41
2:A:316:TYR:CG	2:A:317:LYS:N	2.88	0.41
2:B:155:MET:HE3	2:B:201:GLN:HE22	1.85	0.41
2:A:315:LYS:HD3	2:A:318:ASP:O	2.20	0.41
2:B:57:TYR:HB2	2:B:59:CYS:SG	2.61	0.41
2:B:88:VAL:CG1	2:B:218:LEU:HG	2.50	0.41
2:B:220:ASP:HB3	2:B:221:SER:H	1.63	0.41
2:B:111:LEU:HA	2:B:138:GLY:O	2.20	0.41
1:D:4:DG:O5'	2:B:305:ARG:NH1	2.51	0.41
2:A:90:PRO:CG	2:A:127:PRO:HA	2.39	0.41
2:A:173:LEU:C	2:A:175:TYR:N	2.77	0.41
2:B:222:THR:HG22	2:B:223:GLY:N	2.36	0.41
2:A:286:GLU:CG	2:A:291:VAL:HA	2.42	0.40
2:B:327:VAL:HG22	2:B:345:PHE:HB3	2.02	0.40
2:A:277:ASP:OD2	2:A:333:ARG:HG2	2.21	0.40
2:A:284:GLU:HB3	2:A:292:TRP:HB3	2.02	0.40
2:B:75:ASN:O	2:B:76:LYS:HB2	2.21	0.40
2:B:205:MET:HB2	2:B:205:MET:HE3	1.78	0.40
2:B:283:TYR:OH	2:B:342:PRO:CB	2.69	0.40
1:C:7:DT:H2''	1:C:8:DT:H5''	2.04	0.40
2:A:218:LEU:CD1	2:A:229:LEU:HD21	2.48	0.40
2:B:116:CYS:HA	2:B:121:CYS:HA	2.03	0.40
2:B:327:VAL:HG23	2:B:345:PHE:HB3	2.03	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	
2	A	310/325 (95%)	257 (83%)	35 (11%)	18 (6%)	1	0
2	B	310/325 (95%)	251 (81%)	39 (13%)	20 (6%)	1	0
All	All	620/650 (95%)	508 (82%)	74 (12%)	38 (6%)	1	0

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	87	TYR
2	A	172	ASP
2	A	261	THR
2	A	317	LYS
2	A	322	THR
2	B	71	SER
2	B	76	LYS
2	B	136	ASN
2	B	177	GLN
2	B	188	ASP
2	B	319	VAL
2	A	175	TYR
2	A	176	LEU
2	A	287	GLU
2	B	87	TYR
2	B	88	VAL
2	B	126	GLY
2	B	349	PRO
2	A	89	GLY
2	A	178	ALA
2	B	178	ALA
2	A	174	ALA
2	A	221	SER
2	B	176	LEU
2	B	190	GLU
2	B	220	ASP
2	B	234	SER
2	B	323	LYS
2	A	171	SER
2	A	219	PRO
2	B	320	ASN

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Mol	Chain	Res	Type
2	A	181	GLY
2	A	263	GLY
2	B	223	GLY
2	A	169	VAL
2	A	324	PRO
2	B	160	ILE
2	B	291	VAL

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	
2	A	268/281 (95%)	229 (85%)	39 (15%)	3	3
2	B	268/281 (95%)	233 (87%)	35 (13%)	4	4
All	All	536/562 (95%)	462 (86%)	74 (14%)	3	4

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	41	TYR
2	A	76	LYS
2	A	79	TYR
2	A	87	TYR
2	A	88	VAL
2	A	103	ASN
2	A	111	LEU
2	A	114	LYS
2	A	117	GLU
2	A	132	VAL
2	A	136	ASN
2	A	137	LEU
2	A	149	GLU
2	A	151	LEU
2	A	157	GLU
2	A	167	LEU

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Mol	Chain	Res	Type
2	A	175	TYR
2	A	176	LEU
2	A	185	GLN
2	A	186	LEU
2	A	189	ARG
2	A	192	GLU
2	A	210	VAL
2	A	213	MET
2	A	222	THR
2	A	226	THR
2	A	230	GLU
2	A	235	ASP
2	A	241	LYS
2	A	248	LEU
2	A	249	LYS
2	A	251	VAL
2	A	264	GLU
2	A	293	GLU
2	A	321	ILE
2	A	322	THR
2	A	332	ARG
2	A	339	THR
2	A	341	GLU
2	B	42	LEU
2	B	46	GLU
2	B	73	GLU
2	B	84	ILE
2	B	86	ASN
2	B	95	VAL
2	B	99	THR
2	B	100	ASN
2	B	103	ASN
2	B	114	LYS
2	B	116	CYS
2	B	121	CYS
2	B	136	ASN
2	B	145	LYS
2	B	168	LEU
2	B	177	GLN
2	B	193	ILE
2	B	196	GLN
2	B	200	GLN

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Mol	Chain	Res	Type
2	B	202	THR
2	B	207	LEU
2	B	209	VAL
2	B	218	LEU
2	B	224	SER
2	B	230	GLU
2	B	248	LEU
2	B	255	ARG
2	B	256	THR
2	B	280	ILE
2	B	285	GLU
2	B	301	THR
2	B	312	LYS
2	B	319	VAL
2	B	321	ILE
2	B	324	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	43	GLN
2	A	50	GLN
2	A	86	ASN
2	A	100	ASN
2	A	109	HIS
2	A	136	ASN
2	A	196	GLN
2	B	43	GLN
2	B	75	ASN
2	B	105	HIS
2	B	107	HIS
2	B	109	HIS
2	B	136	ASN
2	B	141	HIS
2	B	201	GLN
2	B	288	ASN
2	B	330	GLN

5.3.3 RNA ⓘ

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.