



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:05 PM GMT

PDB ID : 1NFK  
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](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.

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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

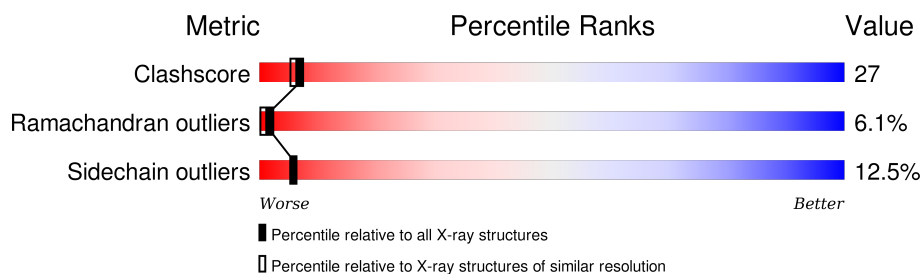
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.


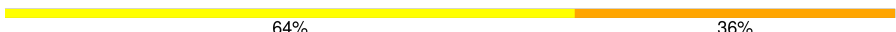


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 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	11	
1	D	11	
2	A	325	
2	B	325	

## 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	A	152	Total	H	O	0	0
			456	304	152		
3	B	114	Total	H	O	0	0
			342	228	114		
3	C	25	Total	H	O	0	0
			75	50	25		
3	D	26	Total	H	O	0	0
			78	52	26		

### 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.

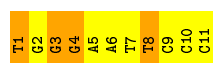
- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*GP\*AP\*AP\*TP\*TP\*CP\*CP\*C)-3')

Chain C: 



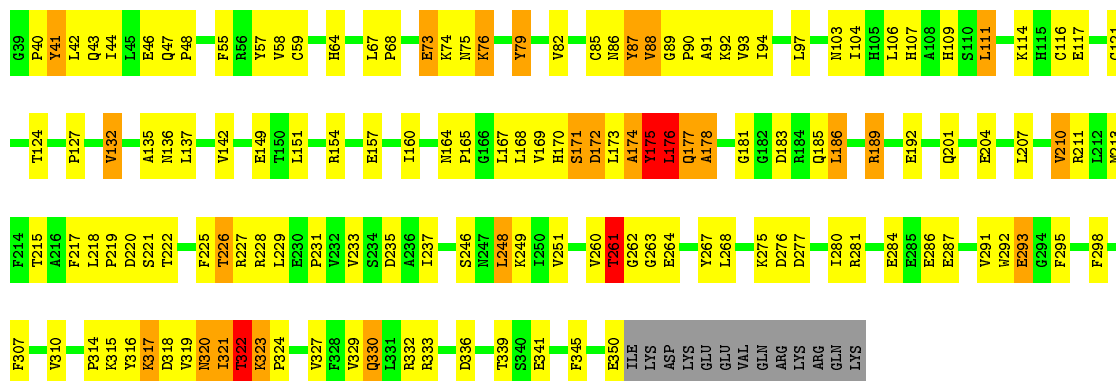
- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*GP\*AP\*AP\*TP\*TP\*CP\*CP\*C)-3')

Chain D: 



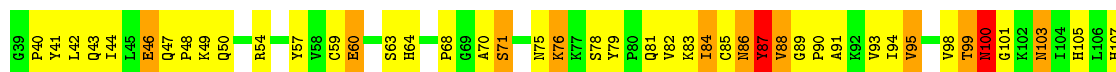
- Molecule 2: PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB))

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 will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.20 Å   132.10 Å   80.10 Å 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 <sup>2</sup> )	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	2.99	26/248 (10.5%)	2.09	11/381 (2.9%)
1	D	3.47	38/248 (15.3%)	2.18	14/381 (3.7%)
2	A	0.60	0/2505	0.89	4/3384 (0.1%)
2	B	0.55	0/2505	0.84	3/3384 (0.1%)
All	All	1.12	64/5506 (1.2%)	1.06	32/7530 (0.4%)

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 (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	DT	C5-C7	12.11	1.57	1.50
1	D	7	DT	C5'-C4'	-11.19	1.39	1.51
1	C	1	DT	N3-C4	-10.50	1.30	1.38
1	D	6	DA	N9-C4	10.27	1.44	1.37
1	C	8	DT	C5'-C4'	-9.51	1.40	1.51
1	D	7	DT	P-O5'	-9.18	1.50	1.59
1	D	8	DT	P-O5'	-9.02	1.50	1.59
1	D	4	DG	C8-N7	8.97	1.36	1.30
1	D	6	DA	C5-C6	-8.93	1.33	1.41
1	C	5	DA	C4'-O4'	8.92	1.53	1.45
1	D	3	DG	N7-C5	8.84	1.44	1.39
1	D	3	DG	C6-N1	-8.83	1.33	1.39
1	C	1	DT	N1-C6	-8.68	1.32	1.38
1	D	8	DT	O3'-P	-8.52	1.50	1.61
1	C	8	DT	C5-C7	-8.15	1.45	1.50
1	D	4	DG	N9-C4	8.02	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	DT	P-O5'	-7.99	1.51	1.59
1	C	4	DG	P-O5'	-7.93	1.51	1.59
1	C	4	DG	C5'-C4'	-7.88	1.42	1.51
1	D	11	DC	N1-C6	-7.85	1.32	1.37
1	D	10	DC	C4'-O4'	-7.66	1.37	1.45
1	C	8	DT	C4-C5	-7.37	1.38	1.45
1	C	8	DT	C2-O2	7.04	1.28	1.22
1	D	5	DA	C4'-O4'	6.83	1.51	1.45
1	D	4	DG	C4'-O4'	6.80	1.51	1.45
1	C	7	DT	C4-C5	-6.78	1.38	1.45
1	D	7	DT	C5-C6	6.76	1.39	1.34
1	D	5	DA	N3-C4	6.67	1.38	1.34
1	D	4	DG	N3-C4	6.59	1.40	1.35
1	D	8	DT	C5'-C4'	-6.54	1.44	1.51
1	D	2	DG	O4'-C1'	6.48	1.50	1.42
1	D	3	DG	C8-N7	6.47	1.34	1.30
1	D	6	DA	C5-C4	-6.46	1.34	1.38
1	C	1	DT	C4'-C3'	-6.31	1.46	1.52
1	C	9	DC	C3'-O3'	-6.29	1.35	1.44
1	D	3	DG	N9-C4	6.23	1.43	1.38
1	C	6	DA	C5'-C4'	6.20	1.58	1.51
1	C	7	DT	C5'-C4'	-6.10	1.44	1.51
1	D	4	DG	C5'-C4'	-6.02	1.44	1.51
1	C	3	DG	N7-C5	5.99	1.42	1.39
1	C	10	DC	C5'-C4'	-5.87	1.44	1.51
1	D	8	DT	N1-C2	5.86	1.42	1.38
1	D	10	DC	C5'-C4'	-5.86	1.45	1.51
1	C	6	DA	N9-C4	5.81	1.41	1.37
1	C	9	DC	C5'-C4'	-5.73	1.45	1.51
1	D	10	DC	C4'-C3'	-5.69	1.46	1.52
1	C	3	DG	C6-O6	5.65	1.29	1.24
1	D	8	DT	C2-N3	-5.61	1.33	1.37
1	C	8	DT	N3-C4	5.61	1.43	1.38
1	D	8	DT	O4'-C1'	5.56	1.49	1.42
1	D	3	DG	O4'-C1'	5.54	1.49	1.42
1	D	7	DT	C3'-O3'	5.24	1.50	1.44
1	C	5	DA	N3-C4	5.22	1.38	1.34
1	D	4	DG	O3'-P	5.20	1.67	1.61
1	D	9	DC	C1'-N1	5.18	1.55	1.49
1	C	3	DG	C5-C6	5.17	1.47	1.42
1	D	8	DT	C3'-O3'	-5.14	1.37	1.44
1	D	4	DG	P-O5'	-5.10	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4	DG	O4'-C1'	-5.06	1.36	1.42
1	D	9	DC	C4'-C3'	-5.06	1.47	1.52
1	C	11	DC	C3'-C2'	-5.05	1.46	1.52
1	D	8	DT	N3-C4	-5.05	1.34	1.38
1	C	4	DG	N3-C4	-5.05	1.31	1.35
1	C	4	DG	C3'-C2'	-5.03	1.46	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	DT	C4-C5-C7	-9.73	113.16	119.00
1	D	5	DA	O4'-C4'-C3'	-7.38	101.55	104.50
1	D	5	DA	O4'-C1'-N9	7.32	113.12	108.00
1	C	11	DC	O4'-C1'-N1	7.18	113.03	108.00
1	C	7	DT	C4-C5-C7	-6.69	114.98	119.00
1	D	1	DT	C4-C5-C7	-6.48	115.11	119.00
1	C	8	DT	C4-C5-C6	6.31	121.78	118.00
1	D	3	DG	O4'-C4'-C3'	-6.23	102.01	104.50
1	D	4	DG	P-O3'-C3'	6.16	127.09	119.70
1	D	4	DG	C8-N9-C4	-6.14	103.95	106.40
1	D	8	DT	C4'-C3'-C2'	6.12	108.61	103.10
2	A	261	THR	N-CA-C	-6.12	94.47	111.00
1	D	1	DT	C4-C5-C6	6.05	121.63	118.00
1	D	4	DG	O4'-C1'-N9	5.81	112.07	108.00
1	C	1	DT	C4-C5-C6	5.80	121.48	118.00
1	C	1	DT	C5-C6-N1	-5.69	120.28	123.70
1	D	8	DT	C4-C5-C7	-5.63	115.62	119.00
1	D	8	DT	C5-C6-N1	-5.63	120.32	123.70
1	C	5	DA	O4'-C4'-C3'	-5.59	102.26	104.50
2	A	248	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	7	DT	C4-C5-C6	5.47	121.28	118.00
2	A	320	ASN	N-CA-C	5.44	125.69	111.00
1	C	5	DA	C4'-C3'-C2'	5.43	107.98	103.10
1	D	8	DT	C4-C5-C6	5.42	121.25	118.00
1	D	2	DG	C4'-C3'-C2'	5.35	107.92	103.10
2	A	268	LEU	CA-CB-CG	5.32	127.53	115.30
2	B	205	MET	N-CA-C	5.26	125.21	111.00
2	B	100	ASN	N-CA-C	-5.20	96.95	111.00
1	C	9	DC	C5'-C4'-C3'	-5.19	104.75	114.10
2	B	60	GLU	N-CA-C	5.14	124.89	111.00
1	C	9	DC	C4'-C3'-C2'	5.10	107.69	103.10
1	D	11	DC	O4'-C1'-C2'	5.01	109.91	105.90

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	121	0
2	B	2453	564	2451	152	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	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 27.

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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:50:GLN:HG3	2:B:236:ALA:O	1.92	0.70
2:A:44:ILE:HA	2:A:82:VAL:HG12	1.73	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
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:B:88:VAL:HB	2:B:218:LEU:HG	1.79	0.64
2:B:42:LEU:HD23	2:B:216:ALA:HB2	1.77	0.64
2:A:310:VAL:HG11	2:B:252:ARG:NH1	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LYS:N	2:B:145:LYS:HD2	2.13	0.63
2:A:211:ARG:HD3	2:A:233:VAL:HG22	1.78	0.63
3:C:33:HOH:O	2:A:57:TYR:HB3	1.98	0.63
2:B:87:TYR:HE1	2:B:89:GLY:HA2	1.65	0.62
2:A:280:ILE:HD12	2:A:298:PHE:CE1	2.35	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:284:GLU:O	2:A:291:VAL:HB	2.03	0.59
2:A:281:ARG:HG3	2:A:295:PHE:CE1	2.37	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:B:44:ILE:HG13	2:B:232:VAL:HG11	1.88	0.56
2:A:75:ASN:O	2:A:76:LYS:HG3	2.06	0.56
2:B:94:ILE:HA	2:B:121:CYS:O	2.05	0.56
2:B:46:GLU:HB3	2:B:81:GLN:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:176:LEU:HD22	2:B:184:ARG:HG2	1.89	0.54
2:A:109:HIS:HE1	2:A:207:LEU:O	1.90	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: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
2:B:281:ARG:NE	2:B:293:GLU:HG3	2.24	0.53
2:B:107:HIS:CE1	2:B:206:ASP:O	2.61	0.53
1:D:3:DG:H1'	1:D:4:DG:H5'	1.89	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:113:GLY:O	2:B:116:CYS:HB2	2.08	0.52
2:B:79:TYR:CD1	2:B:79:TYR:N	2.78	0.52
2:B:148:PHE:HA	2:B:202:THR:HG21	1.91	0.52
2:B:41:TYR:O	2:B:84:ILE:HD12	2.10	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:B:105:HIS:HD2	2:B:168:LEU:O	1.93	0.51
2:A:276:ASP:HB2	3:A:468:HOH:O	2.09	0.51
2:A:217:PHE:HE1	2:A:228:ARG:HB2	1.75	0.51
2:B:184:ARG:HD2	3:B:475:HOH:O	2.10	0.51
2:A:107:HIS:HD2	2:A:109:HIS:H	1.59	0.51
2:B:186:LEU:HB2	2:B:191:LYS:HE3	1.91	0.51
2:A:106:LEU:HD13	2:A:154:ARG:HB3	1.92	0.51
2:A:317:LYS:O	2:A:320:ASN:ND2	2.44	0.51
2:A:307:PHE:CD1	2:B:305:ARG:HG3	2.46	0.50
1:D:4:DG:OP2	2:B:305:ARG:NH1	2.44	0.50
2:B:164:ASN:N	2:B:165:PRO:HD3	2.27	0.50
2:A:114:LYS:NZ	3:A:438:HOH:O	2.44	0.50
3:D:28:HOH:O	2:B:57:TYR:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:TYR:C	2:B:318:ASP:H	2.13	0.49
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: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:A:174:ALA:O	2:A:175:TYR:C	2.51	0.49
2:B:70:ALA:O	2:B:71:SER:HB3	2.13	0.49
2:B:42:LEU:HD13	2:B:43:GLN:N	2.28	0.49
2:A:228:ARG:NH2	3:A:486:HOH:O	2.46	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:B:218:LEU:HD13	2:B:227:ARG:O	2.12	0.48
2:A:109:HIS:CD2	2:A:142:VAL:H	2.31	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:42:LEU:O	2:A:43:GLN:NE2	2.46	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:109:HIS:CD2	2:B:142:VAL:HG22	2.46	0.48
2:B:87:TYR:CE1	2:B:89:GLY:HA2	2.47	0.48
2:B:160:ILE:HA	2:B:184:ARG:HB3	1.96	0.48
2:A:189:ARG:NH1	3:A:445:HOH:O	2.47	0.48
2:A:217:PHE:CE1	2:A:228:ARG:HB2	2.49	0.47
2:B:155:MET:HE3	2:B:201:GLN:NE2	2.28	0.47
2:A:350:GLU:H	2:A:350:GLU:HG2	1.47	0.47
2:A:171:SER:O	2:A:172:ASP:HB3	2.14	0.47
2:B:46:GLU:OE2	2:B:78:SER:HB2	2.15	0.47
2:A:281:ARG:HD3	2:A:330:GLN:OE1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:LEU:HB3	2:B:232:VAL:HG21	1.97	0.47
2:B:100:ASN:HA	2:B:211:ARG:NE	2.29	0.46
2:A:314:PRO:HA	3:A:428:HOH:O	2.15	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:A:104:ILE:HG13	2:A:104:ILE:O	2.16	0.46
2:B:187:THR:N	2:B:190:GLU:HB3	2.30	0.46
2:B:114:LYS:HE3	2:B:114:LYS:N	2.30	0.46
2:B:98:VAL:HB	2:B:105:HIS:O	2.16	0.46
2:A:91:ALA:HB1	2:A:217:PHE:O	2.16	0.46
2:A:47:GLN:OE1	2:A:48:PRO:HD2	2.14	0.46
2:B:83:LYS:HE2	2:B:83:LYS:HB3	1.76	0.46
2:A:320:ASN:HA	2:A:321:ILE:HD13	1.98	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:B:262:GLY:H	2:B:315:LYS:HA	1.82	0.45
2:B:47:GLN:OE1	2:B:48:PRO:HD2	2.16	0.45
2:B:218:LEU:N	2:B:218:LEU:HD12	2.32	0.45
2:B:144:LYS:HE2	3:B:405:HOH:O	2.15	0.45
2:B:336:ASP:O	2:B:337:LEU:HB2	2.16	0.45
2:A:55:PHE:N	2:A:55:PHE:CD1	2.83	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: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:94:ILE:O	2:A:94:ILE:HG13	2.17	0.45
2:A:261:THR:HG22	2:A:262:GLY:N	2.31	0.45
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: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:A:171:SER:O	2:A:172:ASP:CB	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:176:LEU:HD22	2:A:177:GLN:NE2	2.33	0.43
2:B:176:LEU:HA	2:B:176:LEU:HD23	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:B:218:LEU:HD22	2:B:227:ARG:HE	1.84	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: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:HG2	2:B:76:LYS:O	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:322:THR:O	2:B:323:LYS:CB	2.67	0.42
2:B:63:SER:O	2:B:64:HIS:HB3	2.19	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:229:LEU:HD12	2:B:229:LEU:HA	1.88	0.42
2:B:90:PRO:HB2	2:B:225:PHE:HZ	1.84	0.42
1:D:1:DT:C2	2:A:64:HIS:O	2.73	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
2:B:172:ASP:O	2:B:175:TYR:HE2	2.03	0.41
2:B:317:LYS:O	2:B:317:LYS:HG3	2.19	0.41
2:A:201:GLN:HA	2:A:204:GLU:CG	2.49	0.41
2:B:159:CYS:HB3	2:B:176:LEU:HD13	2.02	0.41
2:A:189:ARG:HH11	2:A:189:ARG:HG3	1.85	0.41
2:B:143:THR:CG2	2:B:145:LYS:HD3	2.51	0.41
2:A:175:TYR:CD1	2:A:175:TYR:N	2.88	0.41
2:B:260:VAL:HG22	2:B:347:TYR:HB3	2.01	0.41
2:B:44:ILE:HA	2:B:82:VAL:HG12	2.02	0.41
2:A:316:TYR:CG	2:A:317:LYS:N	2.88	0.41
2:A:210:VAL:HG12	2:A:237:ILE:HB	2.03	0.41
2:B:101:GLY:C	2:B:103:ASN:H	2.24	0.41
2:A:315:LYS:HD3	2:A:318:ASP:O	2.20	0.41
2:B:88:VAL:CG1	2:B:218:LEU:HG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:HB2	2:B:59:CYS:SG	2.61	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
2:A:90:PRO:CG	2:A:127:PRO:HA	2.39	0.41
1:D:4:DG:O5'	2:B:305:ARG:NH1	2.51	0.41
2:B:222:THR:HG22	2:B:223:GLY:N	2.36	0.41
2:A:316:TYR:O	2:A:317:LYS:C	2.60	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:284:GLU:HB3	2:A:292:TRP:HB3	2.02	0.40
2:B:283:TYR:OH	2:B:342:PRO:CB	2.69	0.40
2:A:277:ASP:OD2	2:A:333:ARG:HG2	2.21	0.40
2:B:75:ASN:O	2:B:76:LYS:HB2	2.21	0.40
2:B:116:CYS:HA	2:B:121:CYS:HA	2.03	0.40
2:A:218:LEU:CD1	2:A:229:LEU:HD21	2.48	0.40
1:C:7:DT:H2"	1:C:8:DT:H5"	2.04	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%)	2	1
2	B	310/325 (95%)	251 (81%)	39 (13%)	20 (6%)	1	0
All	All	620/650 (95%)	508 (82%)	74 (12%)	38 (6%)	2	1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	87	TYR

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Mol	Chain	Res	Type
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
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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	268/281 (95%)	228 (85%)	40 (15%)	4	3
2	B	268/281 (95%)	241 (90%)	27 (10%)	9	11
All	All	536/562 (95%)	469 (88%)	67 (12%)	6	6

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	41	TYR
2	A	73	GLU
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	117	GLU
2	A	132	VAL
2	A	137	LEU
2	A	149	GLU
2	A	151	LEU
2	A	157	GLU
2	A	167	LEU
2	A	175	TYR
2	A	176	LEU
2	A	177	GLN
2	A	183	ASP
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	235	ASP
2	A	248	LEU
2	A	249	LYS
2	A	251	VAL

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Mol	Chain	Res	Type
2	A	264	GLU
2	A	293	GLU
2	A	321	ILE
2	A	322	THR
2	A	323	LYS
2	A	330	GLN
2	A	332	ARG
2	A	339	THR
2	A	341	GLU
2	B	46	GLU
2	B	84	ILE
2	B	86	ASN
2	B	87	TYR
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	196	GLN
2	B	200	GLN
2	B	207	LEU
2	B	224	SER
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	316	TYR
2	B	319	VAL

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

Mol	Chain	Res	Type
2	A	43	GLN
2	A	100	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	107	HIS
2	A	109	HIS
2	A	136	ASN
2	A	164	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

### 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.