



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:34 PM UTC

PDB ID : 1A3Q / pdb_00001a3q
Title : HUMAN NF-KAPPA-B P52 BOUND TO DNA
Authors : Cramer, P.; Larson, C.J.; Verdine, G.L.; Muller, C.W.
Deposited on : 1998-01-23
Resolution : 2.10 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

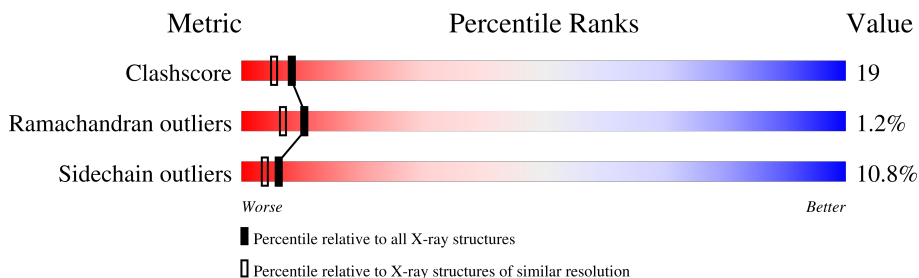
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	82% 18%
2	D	11	64% 36%
3	A	285	55% 37% 7%
3	B	285	52% 37% 9% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5748 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*GP*GP*AP*AP*TP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	P	0	0	0
			222	106	41	65	10			

- Molecule 3 is a protein called PROTEIN (NUCLEAR FACTOR KAPPA-B P52).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	285	Total	C	N	O	S	0	0	0
			2259	1423	409	415	12			
3	B	285	Total	C	N	O	S	0	0	0
			2259	1423	409	415	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ILE	THR	conflict	UNP Q00653
B	213	ILE	THR	conflict	UNP Q00653

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	32	Total	O	0	0
			32	32		
4	D	41	Total	O	0	0
			41	41		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	377	Total 377	O 377	0	0
4	B	335	Total 335	O 335	0	0

3 Residue-property plots [i](#)

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*GP*GP*AP*AP*TP*CP*CP*CP*C)-3')

Chain C: 



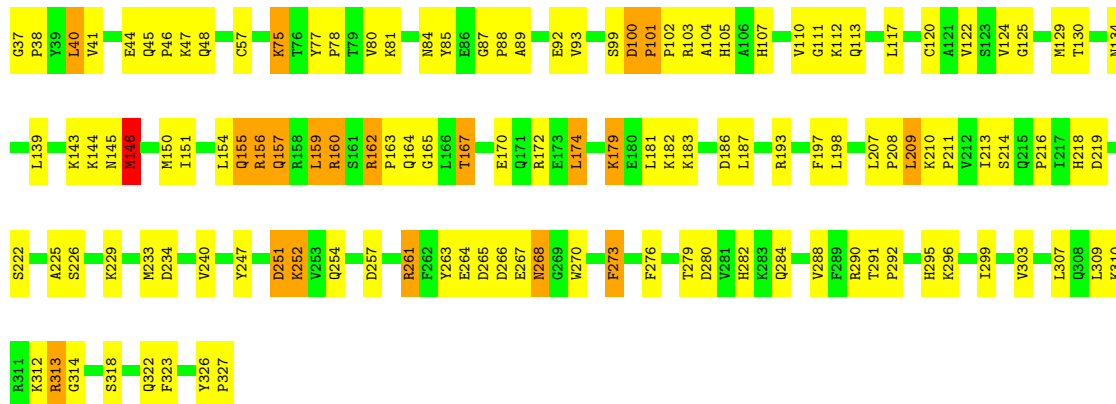
- Molecule 2: DNA (5'-D(*GP*GP*GP*GP*AP*TP*TP*CP*CP*CP*C)-3')

Chain D: 



- Molecule 3: PROTEIN (NUCLEAR FACTOR KAPPA-B P52)

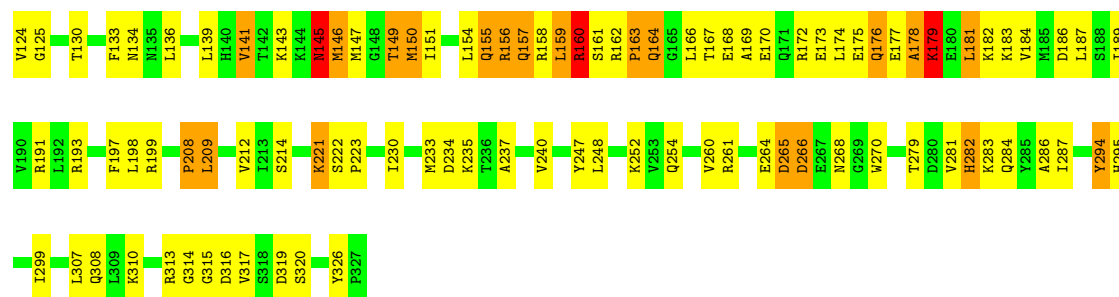
Chain A: 



- Molecule 3: PROTEIN (NUCLEAR FACTOR KAPPA-B P52)

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	44.20Å 121.00Å 134.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.8 (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	6.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.219 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5748	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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	0.53	0/250	0.97	1/384 (0.3%)
2	D	0.52	0/248	1.09	1/381 (0.3%)
3	A	0.78	0/2307	1.28	26/3104 (0.8%)
3	B	0.80	1/2307 (0.0%)	1.31	35/3104 (1.1%)
All	All	0.77	1/5112 (0.0%)	1.27	63/6973 (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
2	D	0	1
3	A	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	233	MET	SD-CE	-6.02	1.64	1.79

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	164	GLN	N-CA-C	15.13	131.12	111.75
3	B	164	GLN	N-CA-C	13.81	129.42	111.75
3	B	100	ASP	N-CA-C	9.85	125.85	112.55
2	D	605	DG	O5'-C5'-C4'	9.78	125.47	110.80
3	B	111	GLY	N-CA-C	9.59	121.19	111.21
3	B	85	TYR	N-CA-C	9.24	123.91	110.42
3	A	111	GLY	N-CA-C	8.32	123.92	112.52
3	B	178	ALA	N-CA-C	-8.28	104.04	114.56
3	A	162	ARG	CA-C-N	8.20	130.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	162	ARG	C-N-CA	8.20	130.09	119.84
1	C	505	DG	O5'-C5'-C4'	8.19	123.08	110.80
3	A	89	ALA	N-CA-C	7.64	120.03	109.18
3	B	100	ASP	CA-C-N	-7.48	112.67	120.38
3	B	100	ASP	C-N-CA	-7.48	112.67	120.38
3	B	181	LEU	N-CA-C	-7.09	104.25	113.12
3	B	89	ALA	N-CA-C	7.08	120.14	109.95
3	A	181	LEU	N-CA-C	-7.04	104.82	113.41
3	B	101	PRO	N-CA-C	-6.77	102.44	110.70
3	B	314	GLY	N-CA-C	6.66	120.95	112.83
3	A	165	GLY	N-CA-C	6.58	120.76	111.42
3	A	101	PRO	N-CA-C	-6.57	102.68	110.70
3	A	174	LEU	N-CA-C	-6.49	103.71	111.69
3	B	155	GLN	N-CA-C	-6.45	103.94	110.97
3	A	209	LEU	N-CA-C	-6.42	100.00	109.81
3	B	221	LYS	N-CA-C	-6.33	106.09	113.88
3	A	164	GLN	CA-C-N	-6.27	116.59	122.17
3	A	164	GLN	C-N-CA	-6.27	116.59	122.17
3	B	179	LYS	N-CA-C	-6.20	104.07	111.69
3	A	37	GLY	CA-C-N	6.19	126.52	119.83
3	A	37	GLY	C-N-CA	6.19	126.52	119.83
3	B	319	ASP	N-CA-C	-6.18	102.38	110.53
3	B	163	PRO	CA-C-N	6.16	129.37	120.38
3	B	163	PRO	C-N-CA	6.16	129.37	120.38
3	B	265	ASP	N-CA-C	6.12	120.72	107.49
3	B	294	TYR	N-CA-C	-6.08	102.34	110.55
3	A	167	THR	N-CA-C	-5.93	102.88	110.53
3	A	155	GLN	N-CA-C	-5.90	104.48	111.03
3	B	48	GLN	N-CA-C	5.84	117.64	111.28
3	B	315	GLY	N-CA-C	-5.82	107.22	115.30
3	B	134	ASN	N-CA-C	5.81	118.08	111.11
3	A	251	ASP	N-CA-C	-5.79	102.74	110.55
3	B	266	ASP	N-CA-C	-5.74	101.08	109.63
3	A	226	SER	N-CA-C	5.62	118.11	110.35
3	B	87	GLY	N-CA-C	5.48	123.51	112.34
3	B	150	MET	N-CA-C	-5.48	105.39	111.36
3	B	133	PHE	CA-C-N	5.42	127.86	120.54
3	B	133	PHE	C-N-CA	5.42	127.86	120.54
3	A	100	ASP	N-CA-C	5.41	121.77	109.81
3	B	169	ALA	N-CA-C	-5.38	105.31	111.07
3	A	146	MET	N-CA-C	5.35	120.19	111.37
3	A	273	PHE	N-CA-C	5.32	117.76	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	209	LEU	N-CA-C	-5.32	101.87	110.32
3	B	282	HIS	N-CA-C	5.23	116.68	109.15
3	B	163	PRO	N-CA-C	5.21	123.21	112.47
3	B	222	SER	CA-C-N	5.18	125.23	119.32
3	B	222	SER	C-N-CA	5.18	125.23	119.32
3	B	208	PRO	N-CA-C	5.17	118.98	110.55
3	A	222	SER	N-CA-C	-5.16	101.91	109.50
3	B	320	SER	N-CA-C	5.14	118.19	109.76
3	A	252	LYS	N-CA-C	5.09	118.18	110.64
3	A	282	HIS	N-CA-C	5.09	116.61	108.41
3	A	134	ASN	N-CA-C	5.09	117.49	111.33
3	A	88	PRO	N-CA-C	-5.04	103.52	111.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	263	TYR	Sidechain
2	D	614	DC	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	223	0	124	2	0
2	D	222	0	125	2	0
3	A	2259	0	2279	90	0
3	B	2259	0	2279	96	0
4	A	377	0	0	13	0
4	B	335	0	0	8	0
4	C	32	0	0	0	0
4	D	41	0	0	1	0
All	All	5748	0	4807	188	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 19.

All (188) 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:B:117:LEU:HD11	3:B:156:ARG:HD2	1.14	1.14
3:A:85:TYR:HB2	3:A:129:MET:HE2	1.57	0.85
3:B:117:LEU:CD1	3:B:156:ARG:HD2	2.04	0.84
3:A:102:PRO:HG3	3:A:213:ILE:HD11	1.62	0.82
3:A:218:HIS:HB3	3:A:225:ALA:HB1	1.60	0.82
3:A:162:ARG:HB3	3:A:163:PRO:HD2	1.63	0.80
3:B:156:ARG:HD3	3:B:160:ARG:HH12	1.47	0.79
3:A:210:LYS:HG3	3:A:211:PRO:HD2	1.67	0.76
3:B:265:ASP:HB3	4:B:2644:HOH:O	1.87	0.75
3:A:45:GLN:OE1	3:A:214:SER:HB2	1.88	0.74
3:A:167:THR:HG22	3:A:170:GLU:HG3	1.71	0.73
3:B:310:LYS:HG3	3:B:317:VAL:HG12	1.70	0.73
3:B:167:THR:HG22	3:B:170:GLU:HG3	1.71	0.73
2:D:612:DC:H2'	3:B:57:CYS:SG	2.29	0.72
3:A:117:LEU:HD11	3:A:156:ARG:HD2	1.72	0.72
3:A:48:GLN:HG3	3:A:216:PRO:O	1.90	0.72
3:B:51:PHE:CD2	3:B:65:LEU:HD12	2.26	0.71
3:B:105:HIS:HD2	3:B:107:HIS:H	1.35	0.71
3:B:159:LEU:HD12	3:B:164:GLN:O	1.90	0.71
3:B:117:LEU:HG	3:B:156:ARG:NH1	2.07	0.69
3:A:103:ARG:HD3	4:A:2493:HOH:O	1.92	0.69
3:B:230:ILE:HG23	3:B:248:LEU:CD1	2.23	0.69
3:B:147:MET:HE1	3:B:179:LYS:HA	1.74	0.69
3:A:313:ARG:HG2	3:A:313:ARG:O	1.92	0.68
3:A:233:MET:HE1	3:A:307:LEU:HD21	1.76	0.67
3:B:158:ARG:HH22	3:B:173:GLU:HG3	1.59	0.67
3:B:240:VAL:HG13	3:B:294:TYR:HB3	1.77	0.66
3:A:229:LYS:HE2	3:A:251:ASP:OD2	1.97	0.65
3:B:237:ALA:HB1	3:B:326:TYR:HE2	1.59	0.65
3:A:117:LEU:HD11	3:A:156:ARG:NH1	2.11	0.64
3:A:85:TYR:CB	3:A:129:MET:HE2	2.26	0.64
3:A:113:GLN:NE2	3:A:122:VAL:HG12	2.12	0.64
3:A:167:THR:HG22	3:A:170:GLU:CG	2.29	0.63
3:B:313:ARG:HG3	4:B:2640:HOH:O	1.97	0.63
3:A:117:LEU:HD11	3:A:156:ARG:CZ	2.29	0.63
3:B:158:ARG:C	3:B:160:ARG:H	2.06	0.63
3:A:117:LEU:CD1	3:A:156:ARG:HD2	2.29	0.62
3:A:105:HIS:HD2	3:A:107:HIS:H	1.47	0.62
3:A:146:MET:SD	3:A:182:LYS:HG3	2.40	0.62
3:B:145:ASN:O	3:B:149:THR:HG23	1.99	0.62
3:B:146:MET:HE2	3:B:187:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:264:GLU:OE2	3:A:295:HIS:HE1	1.82	0.62
3:B:197:PHE:CE2	3:B:208:PRO:HB3	2.34	0.62
3:B:157:GLN:O	3:B:160:ARG:HB2	1.99	0.62
3:A:151:ILE:O	3:A:155:GLN:HG3	2.00	0.61
3:B:237:ALA:HB1	3:B:326:TYR:CE2	2.35	0.61
3:A:117:LEU:HD11	3:A:156:ARG:CD	2.30	0.61
3:B:86:GLU:O	3:B:198:LEU:HD22	2.01	0.60
3:B:158:ARG:HH11	3:B:166:LEU:HD22	1.66	0.60
3:B:44:GLU:HB3	3:B:79:THR:HG23	1.84	0.59
3:A:266:ASP:HB2	3:A:268:ASN:OD1	2.02	0.59
3:A:75:LYS:HE2	3:A:77:TYR:CE1	2.38	0.59
3:A:103:ARG:HE	3:A:104:ALA:H	1.49	0.59
3:A:155:GLN:O	3:A:159:LEU:HD22	2.03	0.58
3:B:77:TYR:O	3:B:79:THR:HG22	2.03	0.58
3:A:240:VAL:HG21	3:A:299:ILE:HG12	1.85	0.58
3:A:160:ARG:HA	3:A:160:ARG:HE	1.69	0.58
3:B:42:ILE:HA	3:B:80:VAL:HG12	1.86	0.57
3:B:230:ILE:HG23	3:B:248:LEU:HD11	1.87	0.57
3:A:92:GLU:HA	3:A:120:CYS:O	2.03	0.57
3:B:240:VAL:HG23	3:B:326:TYR:O	2.05	0.57
3:A:107:HIS:CE1	3:A:187:LEU:HD22	2.40	0.56
3:A:75:LYS:HE2	3:A:77:TYR:HE1	1.71	0.56
3:B:141:VAL:HG22	3:B:145:ASN:HB3	1.88	0.55
3:B:156:ARG:O	3:B:160:ARG:NE	2.40	0.55
3:B:156:ARG:HD3	3:B:160:ARG:NH1	2.18	0.55
3:A:219:ASP:O	3:A:225:ALA:HB3	2.07	0.55
3:A:143:LYS:HE3	4:A:2019:HOH:O	2.07	0.55
3:B:92:GLU:HA	3:B:120:CYS:O	2.07	0.54
3:B:105:HIS:CD2	3:B:107:HIS:H	2.23	0.54
3:A:167:THR:HG23	3:A:170:GLU:H	1.73	0.54
3:B:197:PHE:HE2	3:B:208:PRO:HB3	1.71	0.54
3:A:45:GLN:OE1	3:A:46:PRO:HD2	2.08	0.53
3:B:282:HIS:HB3	3:B:286:ALA:HB3	1.88	0.53
3:A:198:LEU:HD21	3:A:209:LEU:HD11	1.89	0.53
1:C:512:DC:H2'	3:A:57:CYS:SG	2.49	0.53
3:A:261:ARG:HG3	3:A:273:PHE:HE1	1.74	0.52
3:B:155:GLN:O	3:B:159:LEU:HD22	2.09	0.52
3:A:261:ARG:HG3	3:A:273:PHE:CE1	2.44	0.52
3:A:162:ARG:CB	3:A:163:PRO:HD2	2.35	0.52
3:B:235:LYS:NZ	4:B:2417:HOH:O	2.43	0.52
3:B:52:ARG:HG3	3:B:221:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:87:GLY:O	3:B:88:PRO:C	2.53	0.52
3:A:322:GLN:HG3	4:A:2588:HOH:O	2.09	0.52
2:D:610:DT:H72	4:B:2066:HOH:O	2.10	0.51
3:A:234:ASP:HB2	3:A:247:TYR:H	1.74	0.51
3:B:151:ILE:CD1	3:B:175:GLU:HG2	2.41	0.51
3:A:167:THR:CG2	3:A:170:GLU:HG3	2.40	0.51
3:B:264:GLU:HG2	3:B:270:TRP:HE3	1.75	0.51
3:B:93:VAL:HA	3:B:193:ARG:O	2.10	0.51
3:B:155:GLN:HG2	3:B:166:LEU:HD11	1.92	0.51
3:A:117:LEU:CD1	3:A:156:ARG:NH1	2.74	0.50
3:A:81:LYS:HB2	3:A:130:THR:HG22	1.94	0.50
3:A:156:ARG:HA	3:A:159:LEU:HD21	1.92	0.50
3:B:81:LYS:HG3	3:B:130:THR:HG22	1.92	0.50
3:A:87:GLY:HA3	4:A:2554:HOH:O	2.11	0.50
3:B:223:PRO:HB2	3:B:254:GLN:NE2	2.27	0.50
3:B:117:LEU:CD1	3:B:156:ARG:HH11	2.24	0.50
3:A:112:LYS:HE3	4:A:2152:HOH:O	2.12	0.49
3:B:184:VAL:HG12	3:B:184:VAL:O	2.11	0.49
3:A:198:LEU:O	3:A:207:LEU:HB2	2.11	0.49
3:A:264:GLU:HG2	3:A:270:TRP:HE3	1.76	0.49
3:A:257:ASP:HA	3:A:312:LYS:HE2	1.94	0.49
3:B:261:ARG:HD3	3:B:308:GLN:OE1	2.12	0.49
3:B:270:TRP:CG	3:B:295:HIS:HD1	2.30	0.49
3:A:156:ARG:HA	3:A:159:LEU:CD2	2.43	0.49
3:B:81:LYS:NZ	4:B:2639:HOH:O	2.46	0.48
3:B:117:LEU:CG	3:B:156:ARG:NH1	2.74	0.48
3:A:103:ARG:NE	3:A:104:ALA:H	2.09	0.48
3:B:162:ARG:HB3	3:B:163:PRO:HD2	1.96	0.48
3:B:176:GLN:C	3:B:178:ALA:H	2.21	0.48
3:A:198:LEU:HD11	3:A:209:LEU:HD21	1.96	0.47
3:B:38:PRO:O	3:B:209:LEU:HD22	2.14	0.47
3:B:151:ILE:HD11	3:B:175:GLU:HG2	1.96	0.47
3:A:213:ILE:HD12	4:A:2521:HOH:O	2.14	0.47
3:B:117:LEU:CG	3:B:156:ARG:HH11	2.27	0.47
3:A:146:MET:CE	3:A:182:LYS:HG3	2.45	0.47
3:B:283:LYS:HE2	4:B:2453:HOH:O	2.14	0.47
3:B:234:ASP:CG	3:B:247:TYR:HB2	2.40	0.47
3:B:100:ASP:O	3:B:102:PRO:HD3	2.15	0.47
3:B:157:GLN:O	3:B:160:ARG:CB	2.63	0.47
3:B:156:ARG:O	3:B:160:ARG:HD2	2.15	0.46
3:A:210:LYS:HD3	4:A:2479:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:252:LYS:HA	3:A:284:GLN:O	2.15	0.46
3:B:179:LYS:O	3:B:183:LYS:HG2	2.14	0.46
3:B:115:SER:C	3:B:117:LEU:H	2.24	0.46
3:B:234:ASP:HB2	3:B:247:TYR:H	1.80	0.46
3:B:230:ILE:HG23	3:B:248:LEU:HD13	1.95	0.45
3:A:102:PRO:HB3	3:A:213:ILE:HD13	1.97	0.45
3:B:160:ARG:HA	3:B:160:ARG:HE	1.82	0.45
3:B:95:LEU:HG	3:B:109:LEU:HG	1.99	0.45
3:A:290:ARG:HH11	3:A:290:ARG:HG2	1.82	0.45
3:B:83:CYS:O	3:B:84:ASN:HB2	2.17	0.45
3:B:99:SER:O	3:B:191:ARG:NH2	2.49	0.45
3:B:158:ARG:C	3:B:160:ARG:N	2.72	0.45
3:B:264:GLU:OE2	3:B:295:HIS:HE1	2.00	0.44
3:B:45:GLN:OE1	3:B:46:PRO:HD2	2.17	0.44
3:A:276:PHE:HB2	3:A:280:ASP:HB2	1.99	0.44
3:B:156:ARG:HA	3:B:159:LEU:CD2	2.48	0.44
3:B:186:ASP:OD2	3:B:189:ILE:HD12	2.18	0.44
3:A:40:LEU:HG	3:A:41:VAL:N	2.32	0.44
3:B:281:VAL:HG13	3:B:287:ILE:HG12	2.00	0.44
3:A:159:LEU:HD13	4:A:2318:HOH:O	2.18	0.43
3:B:143:LYS:HD2	4:B:2502:HOH:O	2.18	0.43
3:B:42:ILE:HG13	3:B:212:VAL:HG11	2.01	0.43
3:A:309:LEU:HB2	3:A:318:SER:OG	2.18	0.43
3:A:146:MET:O	3:A:150:MET:HB2	2.18	0.43
3:A:179:LYS:O	3:A:183:LYS:HG2	2.19	0.43
3:A:326:TYR:HA	3:A:327:PRO:HD3	1.79	0.43
3:B:45:GLN:OE1	3:B:214:SER:HB2	2.19	0.43
3:A:100:ASP:HB3	3:A:101:PRO:HD3	2.00	0.43
3:B:115:SER:O	3:B:117:LEU:N	2.52	0.42
3:B:146:MET:CE	3:B:182:LYS:HG3	2.49	0.42
3:A:40:LEU:HD11	3:A:80:VAL:HB	2.00	0.42
3:A:117:LEU:HD11	3:A:156:ARG:NE	2.33	0.42
3:B:156:ARG:O	3:B:160:ARG:CD	2.67	0.42
3:A:38:PRO:HG3	3:A:84:ASN:O	2.18	0.42
3:B:177:GLU:O	3:B:181:LEU:HB2	2.19	0.42
3:B:310:LYS:HE3	4:B:2385:HOH:O	2.19	0.42
3:A:291:THR:HG21	3:A:323:PHE:CZ	2.55	0.42
3:B:150:MET:HG3	3:B:181:LEU:HD23	2.00	0.42
1:C:512:DC:H5'	4:D:2010:HOH:O	2.20	0.42
3:A:113:GLN:NE2	4:A:2152:HOH:O	2.50	0.42
3:B:89:ALA:HB3	3:B:124:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:157:GLN:HE21	3:A:157:GLN:HB3	1.65	0.41
3:A:197:PHE:CD1	3:A:208:PRO:HA	2.54	0.41
3:B:240:VAL:CG2	3:B:299:ILE:HD11	2.50	0.41
3:A:40:LEU:HD11	3:A:80:VAL:CG2	2.49	0.41
3:A:280:ASP:HB3	3:A:288:VAL:O	2.21	0.41
3:B:116:GLU:HG2	3:B:116:GLU:O	2.21	0.41
3:A:38:PRO:O	3:A:209:LEU:HD22	2.20	0.41
3:A:156:ARG:HG3	4:A:2470:HOH:O	2.20	0.41
3:B:92:GLU:HG3	3:B:119:ILE:CG2	2.50	0.41
3:B:160:ARG:HB3	3:B:161:SER:H	1.57	0.41
3:A:296:LYS:HE2	4:A:2171:HOH:O	2.19	0.41
3:A:44:GLU:O	3:A:78:PRO:HA	2.21	0.41
3:A:270:TRP:CG	3:A:295:HIS:HD1	2.37	0.41
3:B:72:LYS:HD2	3:B:72:LYS:O	2.21	0.41
3:A:261:ARG:HD2	3:A:310:LYS:HD2	2.02	0.41
3:A:273:PHE:O	3:A:292:PRO:HB3	2.21	0.41
3:A:310:LYS:NZ	4:A:2124:HOH:O	2.54	0.40
3:A:93:VAL:HA	3:A:193:ARG:O	2.21	0.40
3:A:117:LEU:HD13	4:A:2423:HOH:O	2.21	0.40
3:A:105:HIS:HE1	3:A:186:ASP:O	2.05	0.40
3:B:82:ILE:HD12	3:B:124:VAL:HG21	2.03	0.40
3:B:181:LEU:HD12	3:B:181:LEU:HA	1.87	0.40
3:B:252:LYS:HA	3:B:284:GLN:O	2.21	0.40
3:B:136:LEU:HA	3:B:136:LEU:HD23	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	281/285 (99%)	250 (89%)	29 (10%)	2 (1%)	18 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	281/285 (99%)	252 (90%)	24 (8%)	5 (2%)	6	3
All	All	562/570 (99%)	502 (89%)	53 (9%)	7 (1%)	10	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	87	GLY
3	B	125	GLY
3	A	125	GLY
3	B	116	GLU
3	B	145	ASN
3	B	160	ARG
3	A	314	GLY

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	249/249 (100%)	223 (90%)	26 (10%)	7	4
3	B	249/249 (100%)	221 (89%)	28 (11%)	6	3
All	All	498/498 (100%)	444 (89%)	54 (11%)	6	4

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	40	LEU
3	A	47	LYS
3	A	75	LYS
3	A	99	SER
3	A	110	VAL
3	A	124	VAL
3	A	139	LEU
3	A	144	LYS
3	A	145	ASN

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Mol	Chain	Res	Type
3	A	146	MET
3	A	154	LEU
3	A	156	ARG
3	A	157	GLN
3	A	159	LEU
3	A	160	ARG
3	A	172	ARG
3	A	174	LEU
3	A	179	LYS
3	A	254	GLN
3	A	261	ARG
3	A	265	ASP
3	A	267	GLU
3	A	268	ASN
3	A	279	THR
3	A	303	VAL
3	A	313	ARG
3	B	79	THR
3	B	88	PRO
3	B	93	VAL
3	B	100	ASP
3	B	103	ARG
3	B	117	LEU
3	B	139	LEU
3	B	141	VAL
3	B	145	ASN
3	B	146	MET
3	B	149	THR
3	B	154	LEU
3	B	156	ARG
3	B	157	GLN
3	B	159	LEU
3	B	160	ARG
3	B	168	GLU
3	B	172	ARG
3	B	174	LEU
3	B	176	GLN
3	B	179	LYS
3	B	199	ARG
3	B	260	VAL
3	B	266	ASP
3	B	268	ASN

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Mol	Chain	Res	Type
3	B	279	THR
3	B	307	LEU
3	B	316	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	105	HIS
3	A	113	GLN
3	A	134	ASN
3	A	145	ASN
3	A	157	GLN
3	A	164	GLN
3	A	295	HIS
3	A	322	GLN
3	B	98	HIS
3	B	105	HIS
3	B	157	GLN
3	B	176	GLN
3	B	254	GLN
3	B	322	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	1
3	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	199:ARG	C	206:SER	N	6.86
1	B	199:ARG	C	206:SER	N	6.82

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.