Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:52 am BST

PDB ID	:	1NFK
Title	:	STRUCTURE OF THE NUCLEAR FACTOR KAPPA-B (NF-KB) P50 HOMODIMER
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 following versions of software and data (see references ⓘ) were used in the production of this report:

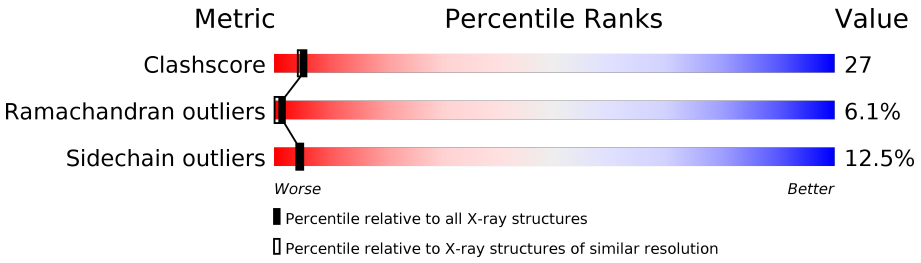
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	11	45% 55%
1	D	11	64% 36%
2	A	325	52% 35% 7%
2	B	325	41% 45% 9%

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		

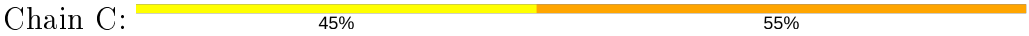
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

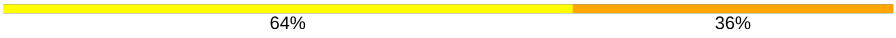
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3')

Chain C:



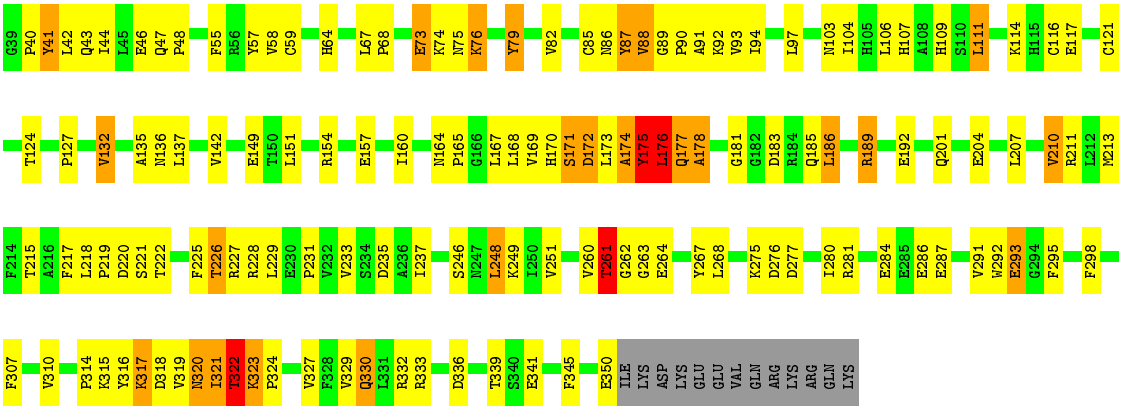
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3')

Chain D:



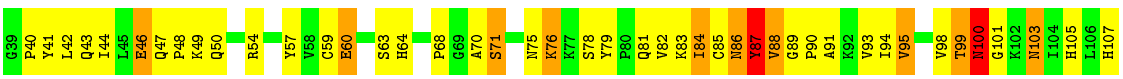
- Molecule 2: PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB))

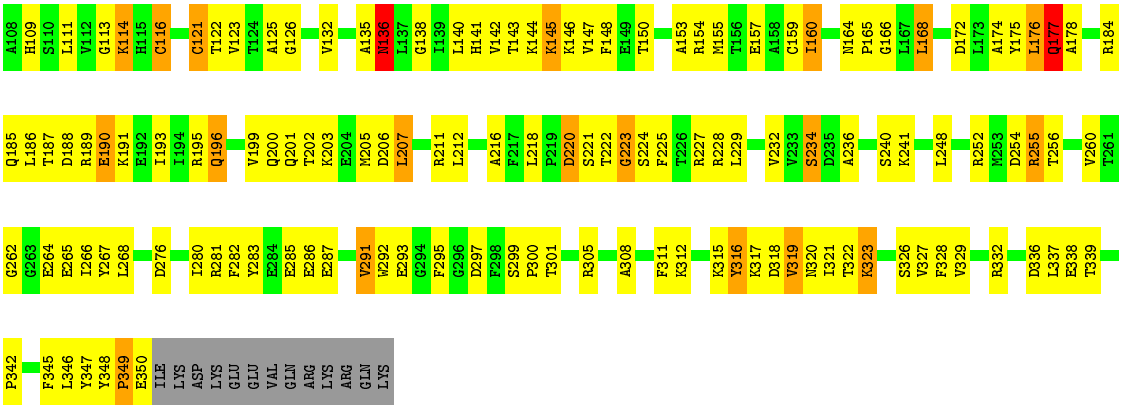
Chain A:



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

Chain B:




A108 H109 S110 L111 V112 G113 K114 H115 C116 C121 T122 V123 T124 A125 G126 V132 A135 N136 L137 G138 I139 L140 H141 V142 T143 K144 K145 K146 V147 F148 E149 T150 A153 R154 M155 T156 E157 A158 C159 I160 N164 P165 G166 L167 L168 D172 L173 A174 Y175 L176 Q177 A178 R184
Q185 L186 T187 D188 R189 E190 K191 E192 I193 I194 R195 Q196 V199 Q200 Q201 T202 K203 E204 M205 D206 L207 R211 L212 A216 F217 L218 P219 D220 S221 T222 G223 S224 F225 T226 R227 R228 L229 V232 V233 S234 D235 A236 S240 K241 L248 R252 M253 D254 R255 T256 V260 T261
G262 G263 E264 E265 I266 Y267 L268 D276 I280 R281 F282 Y283 E284 E285 E286 E287 V291 W292 E293 G294 F295 G296 D297 F298 S299 P300 T301 R305 A308 F311 K312 K315 Y316 K317 D318 V319 N320 I321 T322 K323 S326 V327 F328 V329 R332 D336 L337 E338 T339
P342 F345 L346 Y347 Y348 P349 E350 ILE LYS ASP LYS GLU GLU VAL GLN ARG LYS ARG GLN LYS

4 Data and refinement statistics (i)

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	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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(^{o})	Ideal(^{o})
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 (i)

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

Continued on next page...

Continued from previous page...

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: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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:336:ASP:OD2	2:B:338:GLU:HB2	2.05	0.56
2:B:95:VAL:CG2	2:B:121:CYS:HB2	2.36	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
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:327:VAL:CG2	2:B:345:PHE:HB3	2.36	0.55
2:B:93:VAL:HB	2:B:123:VAL:HG12	1.86	0.55

Continued on next page...

Continued from previous page...

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: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: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: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
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:275:LYS:HG3	2:A:276:ASP:N	2.25	0.51
2:A:73:GLU:OE2	2:A:74:LYS:HD2	2.11	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
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
2:A:114:LYS:NZ	3:A:438:HOH:O	2.44	0.50
2:B:164:ASN:N	2:B:165:PRO:HD3	2.27	0.50
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
3:D:28:HOH:O	2:B:57:TYR:HB3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HA	2:B:190:GLU:OE2	2.11	0.49
2:B:316:TYR:C	2:B:318:ASP:H	2.13	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:174:ALA:O	2:A:175:TYR:C	2.51	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:299:SER:HB3	2:B:300:PRO:HD2	1.95	0.49
2:B:42:LEU:HD13	2:B:43:GLN:N	2.28	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: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: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
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: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

Continued on next page...

Continued from previous page...

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: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:A:104:ILE:HG13	2:A:104:ILE:O	2.16	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:HE3	2:B:114:LYS:N	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: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:A:55:PHE:N	2:A:55:PHE:CD1	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:326:SER:CA	2:B:346:LEU:HD12	2.47	0.45
2:B:42:LEU:HB3	2:B:232:VAL:CG2	2.47	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: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

Continued on next page...

Continued from previous page...

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: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:A:40:PRO:CA	2:A:86:ASN:HB2	2.42	0.43
2:B:218:LEU:HD22	2:B:227:ARG:HE	1.84	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: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:41:TYR:O	2:B:84:ILE:HA	2.19	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
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:O	2:B:317:LYS:HG3	2.19	0.41
2:A:189:ARG:HH11	2:A:189:ARG:HG3	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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASP:HB3	2:B:221:SER:H	1.63	0.41
2:B:57:TYR:HB2	2:B:59:CYS:SG	2.61	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:A:277:ASP:OD2	2:A:333:ARG:HG2	2.21	0.40
2:B:283:TYR:OH	2:B:342:PRO:CB	2.69	0.40
2:B:75:ASN:O	2:B:76:LYS:HB2	2.21	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
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 (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	
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

Continued on next page...

Continued from previous page...

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%)	3 3
2	B	268/281 (95%)	241 (90%)	27 (10%)	7 9
All	All	536/562 (95%)	469 (88%)	67 (12%)	4 5

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

Continued on next page...

Continued from previous page...

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

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.