



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SVC
Title : NFKB P50 HOMODIMER BOUND TO DNA
Authors : Mueller, C.W.; Harrison, S.C.
Deposited on : 1995-11-27
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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
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

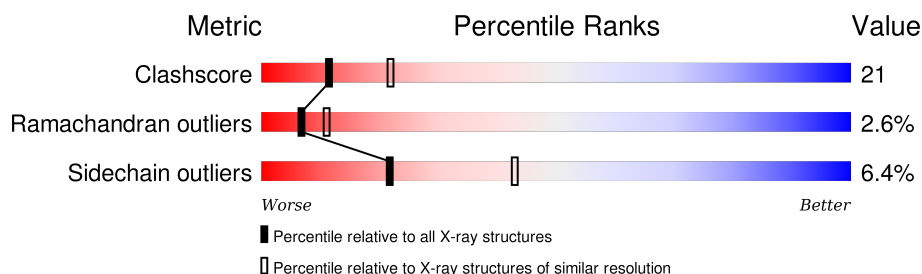
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. 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	D	19	
2	P	365	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2903 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(*AP*GP*AP*TP*GP*GP*GP*GP*AP*AP*TP*CP*CP*CP*CP*TP*A P*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	19	Total	C	N	O	P	0	0	0
			391	186	78	109	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	311	Total	C	N	O	S	0	0	0
			2449	1555	427	456	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	62	ALA	CYS	ENGINEERED	UNP P19838

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	15	Total	O	0	0
			15	15		
3	P	48	Total	O	0	0
			48	48		

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(*AP*GP*AP*TP*GP*GP*GP*GP*AP*AP*TP*CP*CP*CP*CP*TP*A P*GP*A)-3')

Chain D: 

A1 G2 A3 T4 G5 G6 G7 G8 A9 A10 T11 C12 C13 C14 C15 T16 A17 G18 A19

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

Chain P: 

ALA GLU ASP ASP PRO TVR LEU LEU ARG ARG PRO GLU GLN MET PHE HIS LEU ASP PRO SER LEU THR THR ILE PHE ASN PRO GLU VAL PHE GLN PRO GLN MET MET ALA LEU PRO THR ASP GLY P43 Y44 L45 Q46 I47 P51 B54 F58 V61 A62 E63 H67 L70

S74 S75 E76 S81 V85 K86 I87 C88 D89 Y90 V91 G92 P93 A94 G95 V96 I97 V98 Q99 L100 V101 H108 L109 H110 A111 PHE H112 S113 L114 K117 I123 C124 T125 V126 P130 K131 D132 M133 V134 V135 N139 L140 L143 H144 V145 T146 K147 V150 F151 L154

M158 T159 A160 I163 R164 M167 L170 L171 V172 H173 P174 D175 L176 A177 V178 L179 G183 G184 G185 D186 R187 Q188 E193 F194 E195 L196 I197 R198 Q199 A200 A201 Q204 T205 K206 V212 V213 R214 L215 M216 F217 T218 A219 F220 L221 P222 D223 F228 T229 R230 R231 L232

E233 P234 A239 I240 L251 D257 V263 T264 Y270 K278 F285 Y286 E287 E288 E289 E290 V294 M295 E296 G297 P303 T304 T305 D306 V306 H307 R308 A311 K318 Y319 K320 D321 I322 P327 V330 F331 V332 R335 T342 S343 L349 Y350 Y351 P352 E353

ILE LYS ASP LYS GLU GLU VAL GLN ARG LYS ARG ARG GLN LYS

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.00Å 137.00Å 57.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.0 (12.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.225 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2903	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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	D	1.38	0/440	2.68	64/678 (9.4%)
2	P	0.48	0/2502	0.74	0/3379
All	All	0.69	0/2942	1.28	64/4057 (1.6%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	DA	O4'-C1'-N9	9.80	114.86	108.00
1	D	1	DA	N1-C2-N3	-8.71	124.94	129.30
1	D	17	DA	N1-C2-N3	-8.53	125.04	129.30
1	D	9	DA	N1-C2-N3	-8.29	125.15	129.30
1	D	10	DA	N1-C2-N3	-8.23	125.18	129.30
1	D	3	DA	N1-C2-N3	-8.10	125.25	129.30
1	D	19	DA	N1-C2-N3	-8.03	125.29	129.30
1	D	17	DA	C6-N1-C2	7.92	123.35	118.60
1	D	19	DA	C1'-O4'-C4'	-7.85	102.25	110.10
1	D	9	DA	C6-N1-C2	7.80	123.28	118.60
1	D	3	DA	C6-N1-C2	7.74	123.24	118.60
1	D	3	DA	C4'-C3'-C2'	7.72	110.04	103.10
1	D	19	DA	C6-N1-C2	7.71	123.22	118.60
1	D	1	DA	C6-N1-C2	7.68	123.21	118.60
1	D	10	DA	C6-N1-C2	7.67	123.20	118.60
1	D	4	DT	C2-N3-C4	-7.23	122.86	127.20
1	D	1	DA	O4'-C1'-C2'	7.22	111.68	105.90
1	D	16	DT	C2-N3-C4	-7.22	122.87	127.20
1	D	11	DT	C2-N3-C4	-7.20	122.88	127.20
1	D	1	DA	C4'-C3'-C2'	7.14	109.53	103.10
1	D	7	DG	C4'-C3'-C2'	6.83	109.25	103.10
1	D	16	DT	C4'-C3'-C2'	6.73	109.16	103.10
1	D	15	DC	C4'-C3'-C2'	6.71	109.14	103.10
1	D	10	DA	C5-C6-N1	-6.66	114.37	117.70
1	D	17	DA	C4'-C3'-C2'	6.59	109.03	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	DA	O4'-C1'-C2'	6.57	111.16	105.90
1	D	10	DA	C4'-C3'-C2'	6.50	108.95	103.10
1	D	5	DG	O4'-C1'-C2'	6.44	111.05	105.90
1	D	4	DT	C4'-C3'-C2'	6.42	108.88	103.10
1	D	18	DG	C5-C6-N1	6.30	114.65	111.50
1	D	6	DG	C5-C6-N1	6.30	114.65	111.50
1	D	11	DT	P-O3'-C3'	6.18	127.12	119.70
1	D	12	DC	C4'-C3'-C2'	6.17	108.65	103.10
1	D	13	DC	C4'-C3'-C2'	6.11	108.60	103.10
1	D	9	DA	C5-C6-N1	-6.08	114.66	117.70
1	D	11	DT	N1-C2-N3	6.04	118.23	114.60
1	D	13	DC	N3-C4-C5	-6.02	119.49	121.90
1	D	9	DA	C4'-C3'-C2'	5.98	108.48	103.10
1	D	3	DA	C5-C6-N1	-5.94	114.73	117.70
1	D	8	DG	C5-C6-N1	5.89	114.45	111.50
1	D	15	DC	O4'-C1'-C2'	5.83	110.56	105.90
1	D	2	DG	C5-C6-N1	5.82	114.41	111.50
1	D	15	DC	N3-C4-C5	-5.79	119.58	121.90
1	D	19	DA	C5-C6-N1	-5.71	114.84	117.70
1	D	10	DA	O4'-C1'-C2'	5.68	110.44	105.90
1	D	2	DG	C4'-C3'-C2'	5.65	108.19	103.10
1	D	6	DG	C4'-C3'-C2'	5.64	108.18	103.10
1	D	16	DT	O4'-C1'-C2'	5.64	110.41	105.90
1	D	17	DA	C5-C6-N1	-5.61	114.89	117.70
1	D	16	DT	N1-C2-N3	5.59	117.95	114.60
1	D	1	DA	C5-C6-N1	-5.56	114.92	117.70
1	D	7	DG	C5-C6-N1	5.56	114.28	111.50
1	D	5	DG	C5-C6-N1	5.55	114.28	111.50
1	D	7	DG	O4'-C1'-C2'	5.45	110.26	105.90
1	D	4	DT	N1-C2-N3	5.38	117.83	114.60
1	D	8	DG	P-O3'-C3'	5.38	126.16	119.70
1	D	12	DC	N3-C4-C5	-5.38	119.75	121.90
1	D	4	DT	N3-C4-C5	5.36	118.42	115.20
1	D	4	DT	O4'-C1'-C2'	5.30	110.14	105.90
1	D	16	DT	N3-C4-C5	5.27	118.36	115.20
1	D	5	DG	C4'-C3'-C2'	5.26	107.84	103.10
1	D	18	DG	P-O3'-C3'	5.20	125.94	119.70
1	D	6	DG	P-O3'-C3'	5.19	125.93	119.70
1	D	11	DT	C1'-O4'-C4'	-5.07	105.03	110.10

There are no chirality outliers.

There are no planarity outliers.

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	D	391	0	214	15	0
2	P	2449	0	2453	101	0
3	D	15	0	0	1	0
3	P	48	0	0	1	0
All	All	2903	0	2667	113	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 21.

All (113) 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)
2:P:45:LEU:HD12	2:P:219:ALA:HB2	1.39	1.05
2:P:123:ILE:HD12	2:P:164:ARG:HH11	1.46	0.81
2:P:110:HIS:HD2	2:P:112:HIS:H	1.29	0.80
2:P:173:HIS:HD2	2:P:175:ASP:H	1.28	0.80
2:P:218:THR:HG23	2:P:234:PRO:HG3	1.65	0.77
2:P:91:VAL:HG11	2:P:221:LEU:HD13	1.65	0.77
2:P:151:PHE:HA	2:P:205:THR:HG21	1.65	0.76
2:P:201:ALA:O	2:P:205:THR:HG23	1.88	0.73
1:D:15:DC:H2'	1:D:16:DT:C6	2.27	0.70
2:P:158:MET:HE2	2:P:172:VAL:HG13	1.74	0.69
2:P:91:VAL:HB	2:P:221:LEU:HD22	1.74	0.69
2:P:97:ILE:HG22	2:P:125:THR:HG23	1.78	0.66
2:P:117:LYS:HG2	2:P:139:ASN:HB2	1.77	0.66
2:P:61:VAL:HG23	3:P:429:HOH:O	1.97	0.65
2:P:43:PRO:O	2:P:232:LEU:HD22	1.98	0.64
1:D:18:DG:H1'	1:D:19:DA:H4'	1.80	0.63
2:P:263:VAL:HG13	2:P:319:TYR:HB3	1.81	0.62
2:P:91:VAL:HG12	2:P:92:GLY:H	1.65	0.61
2:P:307:HIS:HB3	2:P:311:ALA:HB3	1.83	0.61
2:P:163:ILE:CG2	2:P:185:GLY:HA2	2.31	0.60
2:P:154:LEU:HD12	2:P:205:THR:HG22	1.82	0.60
2:P:231:ARG:HD3	2:P:232:LEU:O	2.02	0.59
2:P:178:TYR:CE1	2:P:179:LEU:HG	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:117:LYS:HG2	2:P:139:ASN:CB	2.32	0.59
1:D:8:DG:OP2	2:P:308:ARG:HD2	2.02	0.59
2:P:123:ILE:HD12	2:P:164:ARG:NH1	2.18	0.58
2:P:43:PRO:HA	2:P:89:ASN:HB2	1.84	0.58
2:P:288:GLU:HG2	2:P:294:VAL:HG12	1.86	0.58
2:P:163:ILE:HG21	2:P:185:GLY:HA2	1.86	0.57
2:P:257:ASP:HB2	2:P:270:TYR:H	1.68	0.57
2:P:154:LEU:O	2:P:158:MET:HG3	2.05	0.56
2:P:167:ASN:ND2	2:P:234:PRO:HG2	2.20	0.56
2:P:221:LEU:HD11	2:P:232:LEU:HD21	1.88	0.55
2:P:110:HIS:CD2	2:P:112:HIS:H	2.17	0.55
2:P:219:ALA:O	2:P:231:ARG:HA	2.06	0.55
2:P:91:VAL:HG12	2:P:92:GLY:N	2.21	0.55
2:P:100:LEU:HG	2:P:114:LEU:HG	1.88	0.55
1:D:2:DG:H2''	1:D:3:DA:OP2	2.07	0.54
2:P:97:ILE:O	2:P:217:PHE:HA	2.07	0.54
1:D:4:DT:H2''	1:D:5:DG:H5''	1.89	0.54
2:P:176:LEU:HD21	2:P:196:LEU:HD12	1.90	0.53
2:P:87:ILE:CD1	2:P:94:ALA:HB3	2.39	0.53
2:P:173:HIS:CD2	2:P:175:ASP:HB2	2.44	0.53
2:P:285:PHE:HA	2:P:331:PHE:O	2.09	0.53
2:P:112:HIS:ND1	2:P:145:VAL:HG12	2.25	0.52
2:P:159:THR:HA	2:P:197:ILE:HD13	1.92	0.52
2:P:327:PRO:HB2	2:P:349:LEU:HD11	1.92	0.51
2:P:45:LEU:HD12	2:P:219:ALA:CB	2.27	0.51
2:P:286:TYR:HA	2:P:295:TRP:O	2.11	0.51
2:P:98:VAL:HB	2:P:124:CYS:HB3	1.93	0.50
2:P:109:LEU:HG	2:P:171:LEU:HB3	1.92	0.50
2:P:92:GLY:O	2:P:94:ALA:N	2.45	0.50
2:P:144:HIS:HD2	2:P:145:VAL:O	1.95	0.50
2:P:251:LEU:HB3	2:P:343:SER:HB3	1.94	0.49
2:P:222:PRO:HA	2:P:228:PHE:HA	1.95	0.49
2:P:287:GLU:HB2	2:P:330:VAL:HG12	1.95	0.49
2:P:183:GLY:O	2:P:188:GLN:HB3	2.13	0.49
2:P:110:HIS:CD2	2:P:111:ALA:N	2.80	0.49
2:P:223:ASP:OD2	2:P:230:ARG:HG2	2.12	0.49
2:P:285:PHE:HB2	2:P:297:GLY:O	2.13	0.48
2:P:319:TYR:CG	2:P:320:LYS:N	2.82	0.48
2:P:335:ARG:HG3	2:P:342:THR:HG22	1.96	0.48
1:D:9:DA:H2''	1:D:10:DA:C8	2.48	0.48
1:D:3:DA:H2''	1:D:4:DT:O5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:318:LYS:HE3	2:P:322:ILE:HD11	1.95	0.47
2:P:94:ALA:HB2	2:P:221:LEU:HD23	1.97	0.47
2:P:167:ASN:HD21	2:P:234:PRO:HG2	1.80	0.47
1:D:10:DA:H5''	2:P:147:LYS:NZ	2.29	0.47
2:P:58:PHE:N	2:P:58:PHE:CD1	2.81	0.47
2:P:74:SER:HB2	2:P:76:GLU:HG2	1.97	0.47
2:P:46:GLN:CG	2:P:47:ILE:N	2.78	0.46
2:P:212:VAL:CG2	2:P:239:ALA:HB1	2.46	0.46
2:P:108:HIS:CD2	2:P:204:GLN:OE1	2.68	0.46
2:P:285:PHE:CE2	2:P:332:VAL:HG22	2.52	0.45
2:P:51:PRO:HG3	2:P:215:LEU:HD12	1.98	0.45
2:P:278:LYS:HA	2:P:306:VAL:HG21	1.99	0.45
2:P:110:HIS:CD2	2:P:111:ALA:H	2.35	0.45
2:P:319:TYR:HD2	2:P:321:ASP:O	1.99	0.45
1:D:18:DG:H2''	1:D:19:DA:O5'	2.16	0.45
2:P:195:GLU:O	2:P:199:GLN:HG2	2.17	0.44
1:D:15:DC:H2'	1:D:16:DT:C5	2.53	0.44
2:P:101:VAL:CG2	2:P:214:ARG:HB2	2.48	0.44
1:D:1:DA:C2'	1:D:2:DG:H5'	2.48	0.43
2:P:173:HIS:CD2	2:P:175:ASP:H	2.19	0.43
2:P:285:PHE:O	2:P:296:GLU:HA	2.17	0.43
3:D:427:HOH:O	2:P:144:HIS:HE1	2.02	0.43
2:P:93:PRO:HG3	2:P:130:PRO:HG3	2.01	0.43
2:P:96:VAL:HG23	2:P:126:VAL:HG13	1.99	0.42
2:P:117:LYS:CG	2:P:139:ASN:HB2	2.46	0.42
1:D:4:DT:C2'	1:D:5:DG:H5''	2.49	0.42
2:P:163:ILE:HG23	2:P:185:GLY:HA2	1.99	0.42
1:D:5:DG:H2''	1:D:6:DG:O5'	2.19	0.42
2:P:63:GLU:O	2:P:67:HIS:NE2	2.50	0.42
1:D:10:DA:H5''	2:P:147:LYS:HZ2	1.84	0.42
2:P:351:TYR:HB2	2:P:352:PRO:HD2	2.01	0.42
2:P:318:LYS:HE3	2:P:322:ILE:CD1	2.50	0.41
1:D:1:DA:O4'	1:D:1:DA:N3	2.52	0.41
2:P:184:GLY:HA3	2:P:188:GLN:HB2	2.01	0.41
2:P:126:VAL:CG1	2:P:135:VAL:HG11	2.50	0.41
2:P:257:ASP:CB	2:P:270:TYR:H	2.32	0.41
2:P:85:VAL:HG12	2:P:86:LYS:N	2.35	0.41
2:P:70:LEU:HD21	2:P:240:ILE:HD13	2.03	0.41
2:P:61:VAL:CG2	2:P:143:LEU:HD11	2.50	0.41
2:P:263:VAL:HG12	2:P:322:ILE:HD13	2.02	0.41
2:P:278:LYS:HB3	2:P:306:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:158:MET:HB2	2:P:197:ILE:HG23	2.02	0.41
2:P:150:VAL:HG12	2:P:205:THR:HB	2.02	0.41
2:P:126:VAL:HG13	2:P:135:VAL:HG11	2.02	0.41
2:P:263:VAL:HG13	2:P:319:TYR:CB	2.47	0.41
2:P:185:GLY:C	2:P:187:ARG:H	2.24	0.41
2:P:140:LEU:HD23	2:P:140:LEU:HA	1.92	0.41
2:P:101:VAL:HG23	2:P:214:ARG:HB2	2.02	0.40
2:P:318:LYS:HG2	2:P:319:TYR:N	2.36	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	P	309/365 (85%)	273 (88%)	28 (9%)	8 (3%)	7 11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	81	SER
2	P	90	TYR
2	P	93	PRO
2	P	290	GLU
2	P	184	GLY
2	P	185	GLY
2	P	89	ASN
2	P	278	LYS

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	P	266 /315 (84%)	249 (94%)	17 (6%)	22	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	54	ARG
2	P	90	TYR
2	P	96	VAL
2	P	125	THR
2	P	132	ASP
2	P	133	MET
2	P	154	LEU
2	P	160	GLU
2	P	170	LEU
2	P	188	GLN
2	P	193	GLU
2	P	206	LYS
2	P	229	THR
2	P	231	ARG
2	P	264	THR
2	P	303	PRO
2	P	304	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	89	ASN
2	P	108	HIS
2	P	110	HIS
2	P	144	HIS
2	P	167	ASN
2	P	173	HIS
2	P	204	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.