



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:15 pm GMT

PDB ID : 2ELB  
Title : Crystal Structure of the BAR-PH domain of human APPL1  
Authors : Li, J.; Mao, X.; Dong, L.Q.; Liu, F.; Tong, L.  
Deposited on : 2007-03-27  
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](mailto: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.

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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  
Xtrriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

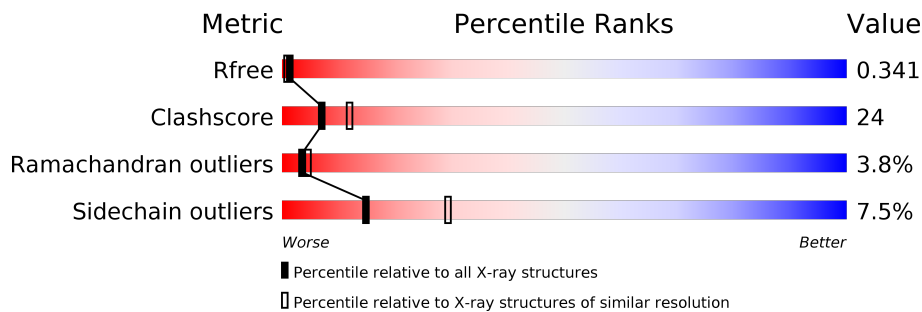
# 1 Overall quality at a glance

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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	396	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2834 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 protein called Adapter protein containing PH domain, PTB domain and leucine zipper motif 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	351	2834	1773	480	561	6	14	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	CLONING ARTIFACT	UNP Q9UKG1
A	-18	GLY	-	CLONING ARTIFACT	UNP Q9UKG1
A	-17	SER	-	CLONING ARTIFACT	UNP Q9UKG1
A	-16	SER	-	CLONING ARTIFACT	UNP Q9UKG1
A	-15	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	-14	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	-13	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	-12	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	-11	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	-10	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	-9	SER	-	CLONING ARTIFACT	UNP Q9UKG1
A	-8	SER	-	CLONING ARTIFACT	UNP Q9UKG1
A	-7	GLY	-	CLONING ARTIFACT	UNP Q9UKG1
A	-6	LEU	-	CLONING ARTIFACT	UNP Q9UKG1
A	-5	VAL	-	CLONING ARTIFACT	UNP Q9UKG1
A	-4	PRO	-	CLONING ARTIFACT	UNP Q9UKG1
A	-3	ARG	-	CLONING ARTIFACT	UNP Q9UKG1
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9UKG1
A	-1	SER	-	CLONING ARTIFACT	UNP Q9UKG1
A	0	HIS	-	CLONING ARTIFACT	UNP Q9UKG1
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	37	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	44	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	82	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	179	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	204	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	213	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	240	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	247	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	270	ASP	LYS	CONFLICT	UNP Q9UKG1
A	310	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	323	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1
A	331	MSE	MET	MODIFIED RESIDUE	UNP Q9UKG1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.57Å 104.13Å 37.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 2.60 29.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.6 (29.84-2.60) 93.1 (29.84-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.327 0.258 , 0.341	Depositor DCC
$R_{free}$ test set	2110 reflections (7.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtrriage
Anisotropy	0.615	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	A	0.45	0/2865	0.62	0/3835

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2834	0	2768	137	0
All	All	2834	0	2768	137	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 24.

All (137) 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:A:330:VAL:HB	1:A:348:ASP:HB2	1.24	1.15
1:A:347:PHE:HA	1:A:351:LYS:HA	1.62	0.81
1:A:18:GLN:HE21	1:A:18:GLN:HA	1.45	0.81
1:A:336:GLU:CD	1:A:337:ASP:H	1.84	0.79
1:A:290:THR:HA	1:A:296:THR:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:H	1:A:186:ASN:HD21	1.31	0.79
1:A:330:VAL:HB	1:A:348:ASP:CB	2.12	0.78
1:A:113:PHE:HB3	1:A:114:PRO:HD3	1.65	0.77
1:A:327:ASN:HD22	1:A:328:CYS:H	1.32	0.74
1:A:7:LEU:HB2	1:A:186:ASN:HD21	1.54	0.72
1:A:309:LEU:O	1:A:325:ILE:HG22	1.89	0.72
1:A:9:ILE:H	1:A:9:ILE:HD12	1.55	0.72
1:A:251:ILE:O	1:A:255:GLU:HB2	1.88	0.72
1:A:102:VAL:HG11	1:A:213:MSE:HE1	1.72	0.71
1:A:225:PHE:CZ	1:A:229:ILE:HD11	2.26	0.70
1:A:359:SER:OG	1:A:362:ASP:HB2	1.90	0.70
1:A:327:ASN:HD22	1:A:328:CYS:N	1.89	0.69
1:A:134:GLN:HE21	1:A:138:ASN:ND2	1.90	0.69
1:A:232:SER:O	1:A:236:VAL:HG23	1.94	0.67
1:A:373:ILE:HG22	1:A:373:ILE:O	1.93	0.67
1:A:332:ALA:O	1:A:333:VAL:HG13	1.93	0.67
1:A:7:LEU:H	1:A:186:ASN:ND2	1.92	0.66
1:A:276:ASN:HA	1:A:372:ASN:HD21	1.61	0.65
1:A:340:TYR:HB2	1:A:343:GLN:NE2	2.11	0.65
1:A:336:GLU:CD	1:A:337:ASP:N	2.51	0.64
1:A:10:GLU:H	1:A:10:GLU:CD	2.02	0.63
1:A:134:GLN:HE21	1:A:138:ASN:HD21	1.45	0.63
1:A:314:ARG:O	1:A:314:ARG:HG2	1.98	0.63
1:A:9:ILE:HG22	1:A:179:MSE:HE2	1.81	0.62
1:A:140:HIS:HA	1:A:170:SER:OG	1.99	0.62
1:A:305:GLN:NE2	1:A:310:MSE:HG3	2.15	0.61
1:A:220:GLU:O	1:A:224:GLU:HG2	2.01	0.61
1:A:248:GLN:O	1:A:252:GLU:HG3	2.02	0.60
1:A:264:PRO:O	1:A:266:PRO:HD3	2.02	0.60
1:A:18:GLN:NE2	1:A:18:GLN:HA	2.14	0.60
1:A:198:GLU:HB3	1:A:199:PRO:HD3	1.84	0.60
1:A:7:LEU:N	1:A:186:ASN:HD21	1.99	0.60
1:A:95:GLU:HG3	1:A:217:ASN:ND2	2.16	0.59
1:A:259:ASP:HA	1:A:262:TYR:CE1	2.38	0.58
1:A:275:ARG:NH1	1:A:364:GLU:OE2	2.37	0.58
1:A:336:GLU:O	1:A:343:GLN:HB2	2.04	0.58
1:A:259:ASP:HA	1:A:262:TYR:CD1	2.40	0.57
1:A:220:GLU:HA	1:A:223:GLU:HG3	1.86	0.57
1:A:372:ASN:C	1:A:374:SER:H	2.08	0.57
1:A:7:LEU:HB2	1:A:186:ASN:ND2	2.19	0.57
1:A:369:THR:O	1:A:373:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:OD1	1:A:299:ARG:HD2	2.06	0.56
1:A:80:GLU:OE1	1:A:81:VAL:N	2.38	0.56
1:A:131:GLU:O	1:A:135:ILE:HG12	2.05	0.56
1:A:287:ARG:HD2	1:A:289:LYS:HD3	1.88	0.56
1:A:133:PHE:HA	1:A:177:THR:HG21	1.89	0.55
1:A:6:LYS:HB3	1:A:26:PHE:HZ	1.71	0.55
1:A:287:ARG:CD	1:A:289:LYS:HD3	2.36	0.55
1:A:280:LYS:HD3	1:A:281:ALA:N	2.22	0.55
1:A:66:LYS:HG2	1:A:66:LYS:O	2.06	0.54
1:A:300:GLN:OE1	1:A:311:SER:HB2	2.08	0.54
1:A:327:ASN:ND2	1:A:328:CYS:N	2.56	0.54
1:A:9:ILE:HG22	1:A:179:MSE:CE	2.38	0.53
1:A:344:ILE:HG22	1:A:367:ILE:HD11	1.90	0.53
1:A:119:LYS:HD3	1:A:119:LYS:O	2.08	0.53
1:A:151:SER:OG	1:A:152:LYS:HE2	2.09	0.52
1:A:336:GLU:OE1	1:A:336:GLU:HA	2.09	0.52
1:A:287:ARG:NE	1:A:289:LYS:HD3	2.25	0.52
1:A:288:ASN:HB2	1:A:338:ARG:HG3	1.92	0.52
1:A:325:ILE:HG23	1:A:326:ASP:N	2.24	0.52
1:A:280:LYS:HD3	1:A:281:ALA:H	1.74	0.52
1:A:285:ASN:HD22	1:A:356:GLN:NE2	2.08	0.52
1:A:274:ASN:C	1:A:274:ASN:HD22	2.13	0.51
1:A:280:LYS:HB3	1:A:366:TRP:CZ3	2.46	0.51
1:A:232:SER:O	1:A:235:ASN:HB2	2.11	0.50
1:A:325:ILE:CG2	1:A:326:ASP:N	2.73	0.50
1:A:340:TYR:HB3	1:A:356:GLN:OE1	2.11	0.50
1:A:88:GLN:HA	1:A:91:LYS:HE2	1.93	0.50
1:A:165:GLU:O	1:A:168:TYR:HB3	2.11	0.50
1:A:88:GLN:HG2	1:A:91:LYS:NZ	2.26	0.50
1:A:357:ALA:HB1	1:A:362:ASP:HB3	1.94	0.50
1:A:288:ASN:OD1	1:A:354:ILE:HD12	2.12	0.50
1:A:314:ARG:H	1:A:314:ARG:HD2	1.76	0.50
1:A:299:ARG:HH11	1:A:299:ARG:HG2	1.77	0.49
1:A:337:ASP:HB2	1:A:343:GLN:HE22	1.78	0.49
1:A:341:CYS:O	1:A:356:GLN:HG3	2.13	0.48
1:A:133:PHE:HA	1:A:177:THR:CG2	2.44	0.48
1:A:333:VAL:HG12	1:A:346:SER:HA	1.94	0.48
1:A:72:ARG:O	1:A:74:PRO:HD3	2.13	0.48
1:A:310:MSE:SE	1:A:324:ASP:HA	2.64	0.47
1:A:327:ASN:ND2	1:A:328:CYS:H	2.08	0.47
1:A:300:GLN:HG2	1:A:313:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:O	1:A:141:ASP:HB2	2.14	0.47
1:A:225:PHE:CE1	1:A:229:ILE:HD11	2.49	0.46
1:A:68:TYR:C	1:A:70:LYS:H	2.18	0.46
1:A:48:TYR:HE2	1:A:108:ALA:HB2	1.80	0.46
1:A:232:SER:HA	1:A:235:ASN:HD22	1.81	0.46
1:A:6:LYS:HB3	1:A:26:PHE:CZ	2.50	0.46
1:A:349:GLY:C	1:A:350:LYS:HD2	2.35	0.46
1:A:274:ASN:CG	1:A:277:LEU:HD13	2.36	0.46
1:A:325:ILE:O	1:A:325:ILE:HD13	2.15	0.46
1:A:373:ILE:O	1:A:373:ILE:CG2	2.62	0.46
1:A:279:ARG:HH11	1:A:279:ARG:HG3	1.82	0.45
1:A:9:ILE:CG2	1:A:179:MSE:HE2	2.45	0.45
1:A:372:ASN:C	1:A:374:SER:N	2.70	0.45
1:A:274:ASN:ND2	1:A:276:ASN:H	2.14	0.45
1:A:274:ASN:HD22	1:A:276:ASN:H	1.65	0.45
1:A:40:LEU:O	1:A:44:MSE:HG3	2.16	0.45
1:A:282:GLY:HA2	1:A:301:PHE:CE1	2.52	0.44
1:A:113:PHE:O	1:A:117:GLN:HG2	2.17	0.44
1:A:22:LEU:HG	1:A:22:LEU:O	2.17	0.44
1:A:180:HIS:O	1:A:183:CYS:HB3	2.18	0.44
1:A:237:ARG:HB2	1:A:237:ARG:NH1	2.32	0.44
1:A:243:ASP:O	1:A:247:MSE:HG3	2.18	0.44
1:A:145:ASN:O	1:A:146:ARG:C	2.56	0.43
1:A:82:MSE:O	1:A:85:THR:HB	2.19	0.43
1:A:9:ILE:HD12	1:A:10:GLU:OE2	2.19	0.43
1:A:178:MSE:HE2	1:A:182:PHE:CE1	2.54	0.43
1:A:337:ASP:HA	1:A:343:GLN:OE1	2.19	0.42
1:A:288:ASN:C	1:A:288:ASN:HD22	2.23	0.42
1:A:273:VAL:HG11	1:A:364:GLU:HG2	2.00	0.42
1:A:37:MSE:HE1	1:A:195:ALA:O	2.18	0.42
1:A:337:ASP:HA	1:A:343:GLN:CD	2.40	0.42
1:A:338:ARG:O	1:A:339:ARG:CB	2.67	0.42
1:A:87:GLN:OE1	1:A:87:GLN:HA	2.20	0.42
1:A:135:ILE:HA	1:A:135:ILE:HD13	1.90	0.42
1:A:212:LYS:HB3	1:A:212:LYS:HE2	1.90	0.42
1:A:360:LYS:HG3	1:A:360:LYS:H	1.60	0.42
1:A:331:MSE:O	1:A:332:ALA:O	2.38	0.41
1:A:259:ASP:N	1:A:260:PRO:HD2	2.35	0.41
1:A:33:ILE:HA	1:A:33:ILE:HD13	1.72	0.41
1:A:305:GLN:O	1:A:308:ASN:HB2	2.21	0.41
1:A:165:GLU:OE1	1:A:165:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:C	1:A:335:CYS:SG	2.98	0.41
1:A:249:GLN:NE2	1:A:253:ASP:OD1	2.51	0.41
1:A:68:TYR:CD2	1:A:86:LEU:HD12	2.56	0.41
1:A:312:GLN:NE2	1:A:317:VAL:HA	2.36	0.41
1:A:334:ASP:O	1:A:335:CYS:SG	2.79	0.41
1:A:201:LEU:O	1:A:205:GLN:HG2	2.20	0.41
1:A:90:SER:O	1:A:94:ASP:HB2	2.22	0.40
1:A:37:MSE:HG3	1:A:118:PHE:CE2	2.56	0.40
1:A:91:LYS:HE2	1:A:91:LYS:HB3	1.86	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
1	A	341/396 (86%)	291 (85%)	37 (11%)	13 (4%)	<b>3</b> <b>4</b>

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ARG
1	A	332	ALA
1	A	351	LYS
1	A	333	VAL
1	A	334	ASP
1	A	336	GLU
1	A	338	ARG
1	A	315	GLY
1	A	329	SER
1	A	339	ARG
1	A	264	PRO
1	A	335	CYS

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Mol	Chain	Res	Type
1	A	69	GLU

### 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
1	A	318/338 (94%)	294 (92%)	24 (8%)	15 29

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	17	PRO
1	A	18	GLN
1	A	33	ILE
1	A	69	GLU
1	A	89	PHE
1	A	274	ASN
1	A	277	LEU
1	A	288	ASN
1	A	289	LYS
1	A	299	ARG
1	A	300	GLN
1	A	314	ARG
1	A	316	ASP
1	A	325	ILE
1	A	326	ASP
1	A	327	ASN
1	A	333	VAL
1	A	336	GLU
1	A	338	ARG
1	A	347	PHE
1	A	350	LYS
1	A	353	SER
1	A	362	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	38	ASN
1	A	51	GLN
1	A	134	GLN
1	A	140	HIS
1	A	175	HIS
1	A	186	ASN
1	A	217	ASN
1	A	221	GLN
1	A	235	ASN
1	A	248	GLN
1	A	274	ASN
1	A	288	ASN
1	A	305	GLN
1	A	312	GLN
1	A	327	ASN
1	A	343	GLN
1	A	356	GLN
1	A	372	ASN

### 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.