



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:25 am BST

PDB ID : 2AEH  
Title : Focal adhesion kinase 1  
Authors : Ceccarelli, D.F.; Song, H.K.; Poy, F.; Schaller, M.D.; Eck, M.J.  
Deposited on : 2005-07-22  
Resolution : 2.53 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

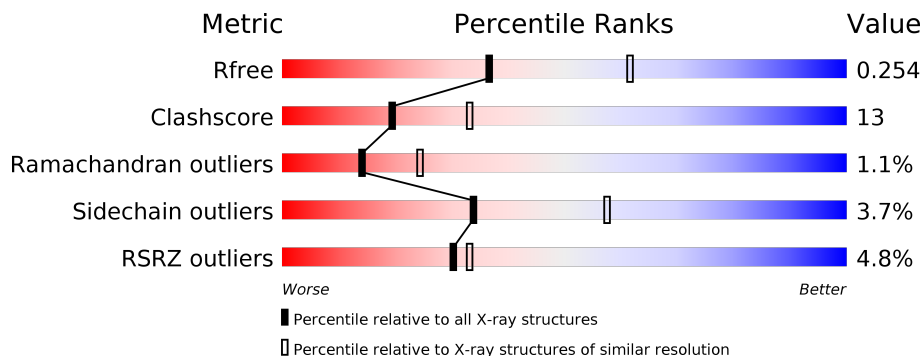
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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))
$R_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	369	 4% 65% 23% 10%
1	B	369	 5% 61% 26% 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5610 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 Focal adhesion kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2685	1714	462	497	12	0	0	0
1	B	331	2682	1712	462	497	11	0	0	0

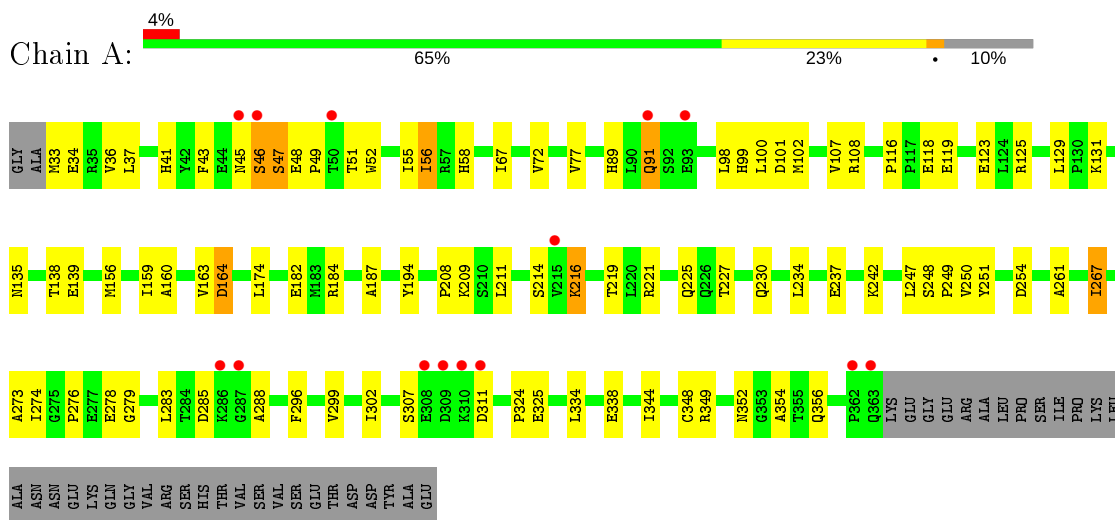
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	127	Total 127	O 127	0	0
2	B	116	Total 116	O 116	0	0

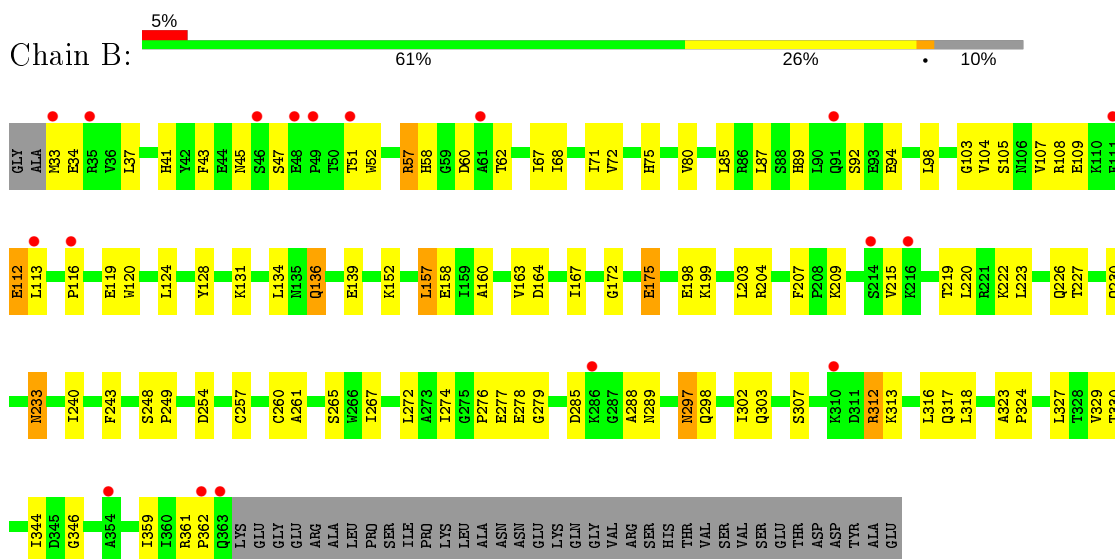
### 3 Residue-property plots [i](#)

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 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.

- Molecule 1: Focal adhesion kinase 1



- Molecule 1: Focal adhesion kinase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.21Å 146.23Å 68.92Å 90.00° 96.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.53 28.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.53) 95.0 (28.59-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.206 , 0.249 0.207 , 0.254	Depositor DCC
$R_{free}$ test set	1472 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtrriage
Anisotropy	0.408	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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	0.41	0/2742	0.59	0/3701
1	B	0.37	0/2739	0.55	0/3698
All	All	0.39	0/5481	0.57	0/7399

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	2685	0	2680	69	0
1	B	2682	0	2673	68	0
2	A	127	0	0	3	0
2	B	116	0	0	6	0
All	All	5610	0	5353	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 13.

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:216:LYS:H	1:A:216:LYS:HD2	1.18	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD22	1:A:100:LEU:H	1.49	0.77
1:B:233:ASN:HD22	1:B:233:ASN:H	1.34	0.73
1:A:33:MET:HG2	1:A:34:GLU:HG2	1.71	0.72
1:A:261:ALA:HB1	1:A:267:ILE:HG23	1.69	0.72
1:A:99:HIS:HB2	1:A:102:MET:HG3	1.72	0.71
1:A:41:HIS:HD2	1:A:43:PHE:H	1.40	0.70
1:B:41:HIS:HD2	1:B:43:PHE:H	1.37	0.70
1:B:316:LEU:HB3	1:B:329:VAL:HB	1.75	0.68
1:B:297:ASN:HD22	1:B:298:GLN:N	1.92	0.66
1:A:98:LEU:HD22	1:A:107:VAL:HG21	1.78	0.65
1:A:216:LYS:N	1:A:216:LYS:HD2	2.02	0.65
1:A:334:LEU:O	1:A:338:GLU:HG3	1.96	0.65
1:B:87:LEU:HD11	1:B:120:TRP:HB3	1.79	0.65
1:B:41:HIS:CD2	1:B:43:PHE:H	2.13	0.65
1:B:261:ALA:HB1	1:B:267:ILE:HG23	1.79	0.64
1:B:108:ARG:O	1:B:112:GLU:HB2	1.97	0.64
1:B:57:ARG:H	1:B:57:ARG:HD2	1.63	0.64
1:B:297:ASN:C	1:B:297:ASN:HD22	2.02	0.63
1:B:265:SER:HB2	2:B:473:HOH:O	1.97	0.63
1:A:100:LEU:CD2	1:A:100:LEU:H	2.12	0.62
1:B:227:THR:O	1:B:230:GLN:HG2	2.01	0.60
1:B:98:LEU:HD22	1:B:107:VAL:HG11	1.83	0.60
1:B:89:HIS:HB3	1:B:92:SER:HB3	1.84	0.59
1:B:152:LYS:HD2	1:B:175:GLU:HG2	1.84	0.59
1:A:307:SER:OG	1:A:311:ASP:HB3	2.02	0.59
1:B:198:GLU:HG3	1:B:199:LYS:HG3	1.85	0.58
1:A:216:LYS:CD	1:A:216:LYS:H	2.01	0.58
1:A:160:ALA:O	1:A:163:VAL:HG12	2.04	0.58
1:B:136:GLN:O	1:B:139:GLU:HG2	2.05	0.57
1:B:67:ILE:O	1:B:71:ILE:HG13	2.04	0.57
1:B:60:ASP:HA	1:B:105:SER:OG	2.05	0.56
1:A:37:LEU:O	1:A:56:ILE:HD13	2.05	0.56
1:A:100:LEU:HD22	1:A:100:LEU:N	2.19	0.56
1:A:116:PRO:HB2	1:A:118:GLU:OE2	2.07	0.55
1:A:56:ILE:HG13	1:A:67:ILE:HD12	1.88	0.55
1:A:138:THR:HG23	1:A:237:GLU:OE2	2.05	0.55
1:B:220:LEU:HA	1:B:223:LEU:HD12	1.89	0.55
1:A:273:ALA:HB2	1:A:283:LEU:HD11	1.88	0.55
1:B:233:ASN:ND2	1:B:233:ASN:H	2.04	0.55
1:B:37:LEU:HD12	2:B:414:HOH:O	2.06	0.54
1:A:285:ASP:HB2	1:A:288:ALA:HB2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:CD2	1:A:43:PHE:H	2.24	0.54
1:A:89:HIS:NE2	1:A:119:GLU:HB3	2.23	0.54
1:A:221:ARG:O	1:A:225:GLN:HG3	2.07	0.53
1:A:299:VAL:HB	1:A:348:CYS:SG	2.49	0.53
1:A:36:VAL:HG13	1:A:55:ILE:HG23	1.90	0.53
1:B:209:LYS:HA	1:B:209:LYS:HE3	1.90	0.53
1:B:222:LYS:O	1:B:226:GLN:HB2	2.10	0.52
1:B:116:PRO:HD2	1:B:119:GLU:OE1	2.10	0.52
1:B:318:LEU:HD11	1:B:344:ILE:HD13	1.91	0.51
1:B:45:ASN:HB2	1:B:52:TRP:CD1	2.45	0.51
1:A:267:ILE:H	1:A:267:ILE:HD12	1.76	0.51
1:A:174:LEU:HD11	1:A:242:LYS:HG3	1.93	0.51
1:B:204:ARG:HG2	1:B:204:ARG:HH11	1.76	0.51
1:B:361:ARG:HB3	1:B:362:PRO:HD2	1.92	0.51
1:A:216:LYS:HE2	2:A:453:HOH:O	2.11	0.51
1:B:257:CYS:HA	1:B:272:LEU:O	2.11	0.51
1:A:139:GLU:HB3	2:A:523:HOH:O	2.11	0.50
1:A:37:LEU:HB3	1:A:56:ILE:HD11	1.93	0.50
1:A:273:ALA:HB2	1:A:283:LEU:CD1	2.42	0.50
1:A:184:ARG:HB2	1:A:187:ALA:HB2	1.93	0.49
1:A:261:ALA:CB	1:A:267:ILE:HG23	2.42	0.49
1:A:72:VAL:HB	1:A:77:VAL:HB	1.95	0.49
1:A:49:PRO:HA	1:A:52:TRP:CE2	2.48	0.49
1:B:92:SER:OG	1:B:94:GLU:HG2	2.12	0.49
1:B:240:ILE:O	1:B:243:PHE:HB3	2.12	0.48
1:A:129:LEU:O	1:A:276:PRO:HB3	2.14	0.48
1:A:285:ASP:HB2	1:A:288:ALA:CB	2.44	0.48
1:B:312:ARG:HH11	1:B:312:ARG:HG3	1.79	0.48
1:B:58:HIS:HB2	1:B:62:THR:OG1	2.14	0.47
1:A:89:HIS:CD2	1:A:119:GLU:HB3	2.50	0.47
1:A:89:HIS:CD2	1:A:91:GLN:H	2.32	0.47
1:A:352:ASN:C	1:A:354:ALA:H	2.18	0.47
1:A:160:ALA:HB1	1:A:208:PRO:HB3	1.97	0.47
1:A:254:ASP:O	1:A:276:PRO:HD2	2.14	0.47
1:B:163:VAL:HG21	1:B:167:ILE:HG21	1.97	0.47
1:B:51:THR:HG22	1:B:51:THR:O	2.15	0.47
1:A:37:LEU:HB3	1:A:56:ILE:CD1	2.44	0.47
1:B:52:TRP:HA	2:B:476:HOH:O	2.14	0.47
1:A:159:ILE:CD1	1:A:251:TYR:HB2	2.45	0.47
1:B:303:GLN:HG3	1:B:317:GLN:HB3	1.97	0.46
1:B:104:VAL:O	1:B:108:ARG:HG3	2.14	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:HG22	1:B:164:ASP:H	1.80	0.46
1:B:215:VAL:CG1	1:B:219:THR:HB	2.45	0.46
1:A:58:HIS:HE1	1:A:108:ARG:HH11	1.64	0.46
1:B:160:ALA:O	1:B:163:VAL:HG12	2.15	0.46
1:B:172:GLY:HA3	1:B:207:PHE:CE2	2.50	0.46
1:A:274:ILE:HA	1:A:279:GLY:O	2.16	0.45
1:B:198:GLU:HA	1:B:203:LEU:HG	1.98	0.45
1:B:33:MET:C	1:B:34:GLU:HG3	2.37	0.45
1:B:285:ASP:HB2	1:B:288:ALA:HB2	1.98	0.45
1:A:194:TYR:CD2	1:A:221:ARG:HG3	2.51	0.45
1:A:156:MET:HA	1:A:160:ALA:HB2	1.99	0.45
1:A:247:LEU:HG	1:A:251:TYR:HB3	1.98	0.45
1:B:72:VAL:HG21	1:B:80:VAL:HG23	1.99	0.45
1:A:46:SER:O	1:A:47:SER:HB3	2.17	0.45
1:A:349:ARG:O	1:A:352:ASN:O	2.35	0.44
1:B:254:ASP:O	1:B:276:PRO:HD2	2.18	0.44
1:A:267:ILE:H	1:A:267:ILE:CD1	2.31	0.44
1:B:103:GLY:O	1:B:107:VAL:HG23	2.17	0.44
1:A:101:ASP:HB3	2:A:415:HOH:O	2.17	0.43
1:A:123:GLU:HG3	1:A:125:ARG:HG3	1.99	0.43
1:B:260:CYS:HB2	1:B:330:THR:O	2.17	0.43
1:A:248:SER:N	1:A:249:PRO:HD2	2.33	0.43
1:A:208:PRO:HG2	1:A:211:LEU:HB2	2.01	0.43
1:B:277:GLU:HB2	2:B:426:HOH:O	2.19	0.43
1:B:109:GLU:O	1:B:113:LEU:HD13	2.19	0.43
1:B:34:GLU:HB3	1:B:58:HIS:O	2.19	0.43
1:B:307:SER:HB2	1:B:313:LYS:HB2	2.00	0.43
1:B:277:GLU:HG2	2:B:436:HOH:O	2.19	0.43
1:B:68:ILE:O	1:B:72:VAL:HG22	2.18	0.43
1:A:227:THR:O	1:A:230:GLN:HG2	2.19	0.43
1:B:274:ILE:HA	1:B:279:GLY:O	2.18	0.43
1:B:89:HIS:CD2	1:B:119:GLU:HB3	2.54	0.43
1:A:45:ASN:O	1:A:46:SER:C	2.57	0.42
1:B:71:ILE:O	1:B:75:HIS:HD2	2.02	0.42
1:B:248:SER:N	1:B:249:PRO:HD2	2.35	0.42
1:B:324:PRO:HG2	2:B:416:HOH:O	2.20	0.42
1:A:267:ILE:HD12	1:A:267:ILE:N	2.33	0.42
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.84	0.42
1:B:157:LEU:C	1:B:158:GLU:HG3	2.40	0.42
1:A:324:PRO:HG2	1:A:325:GLU:H	1.85	0.41
1:B:152:LYS:HD2	1:B:175:GLU:CG	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:CE2	1:A:221:ARG:HG3	2.55	0.41
1:A:250:VAL:HG22	1:A:250:VAL:O	2.19	0.41
1:B:323:ALA:HA	1:B:324:PRO:HD2	1.94	0.41
1:A:159:ILE:HD11	1:A:251:TYR:HB2	2.03	0.41
1:A:302:ILE:HD11	1:A:344:ILE:HG22	2.01	0.41
1:B:128:TYR:CD2	1:B:346:GLY:HA3	2.54	0.41
1:A:279:GLY:HA2	1:A:296:PHE:CE1	2.55	0.41
1:B:302:ILE:O	1:B:359:ILE:HA	2.21	0.40
1:A:209:LYS:C	1:A:211:LEU:H	2.24	0.40
1:A:163:VAL:HG22	1:A:164:ASP:N	2.37	0.40
1:B:312:ARG:NH1	1:B:312:ARG:HG3	2.36	0.40
1:A:216:LYS:HD3	1:A:219:THR:OG1	2.21	0.40
1:A:48:GLU:HB3	1:A:51:THR:HG23	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	
1	A	329/369 (89%)	300 (91%)	24 (7%)	5 (2%)	10	17
1	B	329/369 (89%)	297 (90%)	30 (9%)	2 (1%)	25	41
All	All	658/738 (89%)	597 (91%)	54 (8%)	7 (1%)	14	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	B	47	SER
1	A	214	SER
1	A	47	SER
1	A	131	LYS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	131	LYS
1	A	267	ILE

### 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	294/326 (90%)	285 (97%)	9 (3%)	40	65
1	B	293/326 (90%)	280 (96%)	13 (4%)	28	49
All	All	587/652 (90%)	565 (96%)	22 (4%)	34	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ILE
1	A	91	GLN
1	A	135	ASN
1	A	164	ASP
1	A	182	GLU
1	A	216	LYS
1	A	234	LEU
1	A	278	GLU
1	A	356	GLN
1	B	57	ARG
1	B	85	LEU
1	B	112	GLU
1	B	124	LEU
1	B	136	GLN
1	B	157	LEU
1	B	175	GLU
1	B	233	ASN
1	B	278	GLU
1	B	289	ASN
1	B	297	ASN
1	B	312	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	327	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	45	ASN
1	A	58	HIS
1	A	75	HIS
1	A	89	HIS
1	A	96	HIS
1	A	115	HIS
1	A	135	ASN
1	A	289	ASN
1	A	292	HIS
1	A	303	GLN
1	B	41	HIS
1	B	45	ASN
1	B	75	HIS
1	B	91	GLN
1	B	135	ASN
1	B	136	GLN
1	B	225	GLN
1	B	226	GLN
1	B	233	ASN
1	B	289	ASN
1	B	297	ASN
1	B	303	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	331/369 (89%)	0.03	14 (4%) 36 40	21, 43, 76, 96	0
1	B	331/369 (89%)	0.22	18 (5%) 25 28	28, 51, 86, 99	0
All	All	662/738 (89%)	0.12	32 (4%) 30 33	21, 47, 84, 99	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	LYS	7.5
1	B	362	PRO	5.6
1	B	33	MET	5.0
1	A	286	LYS	4.7
1	B	286	LYS	4.5
1	B	216	LYS	4.3
1	B	113	LEU	4.2
1	A	308	GLU	4.2
1	B	49	PRO	3.9
1	B	51	THR	3.9
1	A	287	GLY	3.7
1	B	310	LYS	3.6
1	B	48	GLU	3.2
1	A	309	ASP	3.1
1	A	215	VAL	3.1
1	A	45	ASN	3.1
1	A	46	SER	3.0
1	B	214	SER	2.9
1	A	362	PRO	2.9
1	A	50	THR	2.6
1	A	91	GLN	2.6
1	B	91	GLN	2.5
1	A	311	ASP	2.5
1	A	363	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	116	PRO	2.3
1	B	46	SER	2.3
1	B	363	GLN	2.2
1	B	61	ALA	2.1
1	B	35	ARG	2.1
1	A	93	GLU	2.1
1	B	111	PHE	2.0
1	B	354	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.