



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:08 am GMT

PDB ID : 2J63  
Title : CRYSTAL STRUCTURE OF AP ENDONUCLEASE LMAP FROM LEISHMANIA MAJOR  
Authors : Vidal, A.E.; Harkiolaki, M.; Gallego, C.; Castillo-Acosta, V.M.; Ruiz-Perez, L.M.; Wilson, K.S.; Gonzalez-Pacanowska, D.  
Deposited on : 2006-09-25  
Resolution : 2.48 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

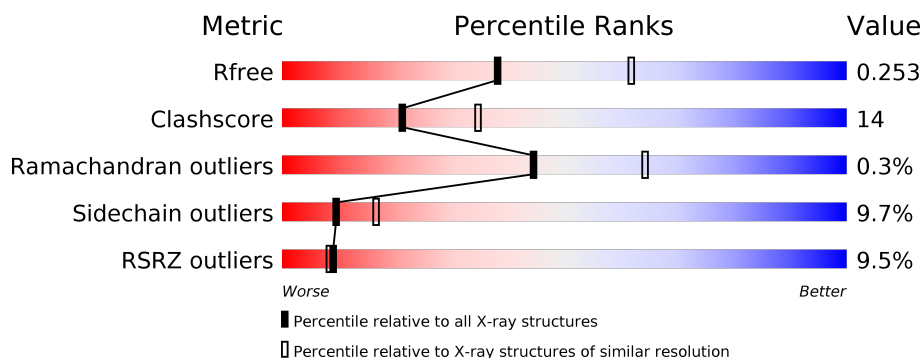
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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))
$R_{free}$	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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  $\leq 5\%$ . 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	467	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>17%</div> <div>•</div> <div>29%</div> </div> </div>
1	B	467	<div> <div>8%</div> <div> <div></div> <div>50%</div> <div>18%</div> <div>•</div> <div>29%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5443 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.

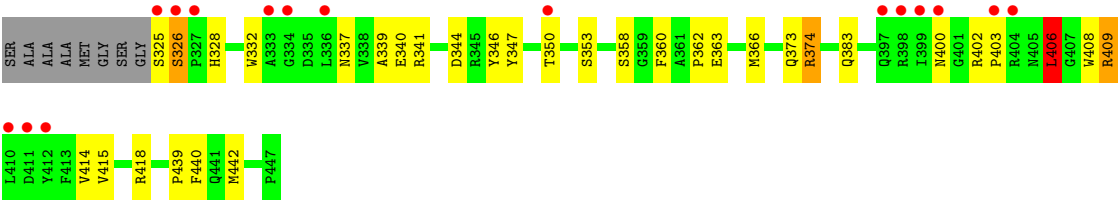
- Molecule 1 is a protein called AP-ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2654	1673	469	494	18			
1	B	333	Total	C	N	O	S	0	0	0
			2654	1673	469	494	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	60	Total	O	0	0
			60	60		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.10Å 45.01Å 115.13Å 90.00° 116.79° 90.00°	Depositor
Resolution (Å)	105.41 – 2.48 29.25 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.2 (105.41-2.48) 99.3 (29.25-2.48)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.246 0.205 , 0.253	Depositor DCC
$R_{free}$ test set	1378 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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

### 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	A	0.59	1/2720 (0.0%)	0.73	4/3682 (0.1%)
1	B	0.58	1/2720 (0.0%)	0.69	3/3682 (0.1%)
All	All	0.59	2/5440 (0.0%)	0.71	7/7364 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	TYR	C-N	-6.70	1.18	1.34
1	A	213	VAL	C-N	-5.64	1.21	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	409	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	409	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	290	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	406	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	262	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	262	ASP	CB-CG-OD2	5.21	122.99	118.30

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	A	2654	0	2558	65	0
1	B	2654	0	2557	77	0
2	A	75	0	0	2	0
2	B	60	0	0	6	0
All	All	5443	0	5115	142	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 14.

All (142) 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:B:374:ARG:HH11	1:B:374:ARG:HG2	1.27	1.00
1:B:141:ARG:HD3	1:B:141:ARG:H	1.28	0.98
1:B:217:HIS:CD2	1:B:261:PRO:HD3	2.04	0.92
1:B:141:ARG:NH1	1:B:142:GLY:H	1.67	0.90
1:B:133:ILE:HD11	1:B:439:PRO:HB3	1.56	0.87
1:A:192:HIS:HB3	1:A:203:THR:HG22	1.56	0.85
1:A:310:THR:HG22	1:A:311:GLU:H	1.45	0.81
1:B:141:ARG:HH11	1:B:142:GLY:H	1.24	0.81
1:A:310:THR:HG22	1:A:311:GLU:N	1.96	0.80
1:B:374:ARG:CG	1:B:374:ARG:HH11	1.97	0.76
1:A:374:ARG:HH11	1:A:374:ARG:HG2	1.49	0.76
1:B:192:HIS:CE1	1:B:250:GLY:HA2	2.20	0.75
1:B:192:HIS:HB3	1:B:203:THR:HG22	1.69	0.74
1:B:347:TYR:HA	2:B:2046:HOH:O	1.87	0.73
1:B:261:PRO:HD2	2:B:2034:HOH:O	1.88	0.72
1:A:310:THR:CG2	1:A:311:GLU:N	2.53	0.71
1:B:344:ASP:OD1	1:B:409:ARG:HD3	1.91	0.70
1:B:133:ILE:HD11	1:B:439:PRO:CB	2.21	0.70
1:A:350:THR:HG23	1:A:353:SER:H	1.56	0.70
1:B:192:HIS:CD2	1:B:222:ARG:HD3	2.28	0.69
1:B:249:GLU:OE1	1:B:251:ARG:NH1	2.26	0.69
1:A:299:ARG:NH1	1:A:371:THR:OG1	2.26	0.68
1:B:166:GLN:HB2	1:B:276:TYR:HB2	1.76	0.68
1:A:209:ASN:O	1:A:214:LYS:HG3	1.94	0.68
1:A:306:ASP:O	1:A:310:THR:HB	1.94	0.66
1:A:249:GLU:OE1	1:A:251:ARG:NH1	2.29	0.65
1:B:279:ASN:HD22	1:B:281:GLY:H	1.42	0.65
1:B:374:ARG:NH1	1:B:374:ARG:HG2	2.03	0.65
1:A:344:ASP:OD1	1:A:409:ARG:HD3	1.97	0.65
1:A:279:ASN:HD22	1:A:281:GLY:H	1.45	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:CG	1:A:374:ARG:HH11	2.11	0.64
1:B:275:THR:CG2	1:B:277:VAL:HG23	2.28	0.63
1:B:228:SER:HB2	1:B:243:GLU:OE2	1.98	0.63
1:B:132:PHE:HD1	1:B:162:VAL:HG13	1.63	0.62
1:B:350:THR:HG23	1:B:353:SER:H	1.64	0.62
1:B:133:ILE:HG13	1:B:134:THR:N	2.14	0.61
1:B:287:LEU:HB3	1:B:288:PRO:HD3	1.83	0.60
1:B:339:ALA:HB1	1:B:344:ASP:HB3	1.82	0.60
1:B:104:SER:HB3	1:B:107:GLU:OE2	2.02	0.60
1:B:251:ARG:NH2	2:B:2032:HOH:O	2.33	0.60
1:A:411:ASP:OD1	1:A:437:HIS:HD2	1.84	0.60
1:A:192:HIS:HB3	1:A:203:THR:CG2	2.30	0.59
1:A:133:ILE:HG13	1:A:134:THR:N	2.17	0.59
1:A:166:GLN:HB2	1:A:276:TYR:HB2	1.84	0.58
1:A:133:ILE:HD11	1:A:439:PRO:HB3	1.84	0.57
1:A:374:ARG:NH1	1:A:374:ARG:HG2	2.19	0.57
1:B:132:PHE:CD1	1:B:162:VAL:HG13	2.40	0.57
1:A:207:MET:HE2	1:A:218:ALA:HB3	1.87	0.56
1:B:133:ILE:HD13	1:B:154:PHE:HZ	1.69	0.56
1:B:140:LEU:HD21	1:B:204:ARG:NH1	2.21	0.56
1:B:279:ASN:ND2	1:B:358:SER:OG	2.37	0.56
1:A:303:HIS:O	1:A:307:THR:HG22	2.05	0.56
1:B:158:GLU:HB3	1:B:160:PRO:HD3	1.87	0.56
1:A:136:ASN:HB3	1:A:437:HIS:CG	2.41	0.55
1:B:141:ARG:N	1:B:141:ARG:HD3	2.11	0.55
1:B:362:PRO:O	1:B:366:MET:HG3	2.07	0.55
1:B:280:SER:OG	1:B:287:LEU:HD23	2.08	0.54
1:A:166:GLN:NE2	2:A:2020:HOH:O	2.40	0.54
1:B:287:LEU:N	1:B:288:PRO:CD	2.70	0.54
1:B:346:TYR:CG	1:B:406:LEU:HB2	2.44	0.52
1:A:404:ARG:HB3	1:A:406:LEU:HD22	1.90	0.52
1:A:351:PHE:O	1:A:355:GLN:HG3	2.09	0.52
1:A:90:ILE:HG23	1:A:91:ARG:HG3	1.91	0.52
1:A:133:ILE:HG12	1:A:163:LEU:HD13	1.92	0.52
1:A:362:PRO:O	1:A:366:MET:HG3	2.10	0.51
1:B:141:ARG:CD	1:B:141:ARG:H	1.96	0.51
1:B:304:ARG:HA	1:B:307:THR:HG22	1.92	0.51
1:B:141:ARG:NH1	1:B:142:GLY:N	2.50	0.51
1:A:207:MET:CE	1:A:218:ALA:HB3	2.41	0.51
1:A:402:ARG:HB3	1:A:403:PRO:HD3	1.92	0.51
1:B:363:GLU:HA	1:B:366:MET:HE2	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:HA	1:A:307:THR:HG23	1.93	0.50
1:A:192:HIS:NE2	1:A:250:GLY:HA2	2.27	0.50
1:B:151:LEU:O	1:B:155:MET:HG2	2.11	0.50
1:B:192:HIS:HE1	1:B:247:ASP:OD1	1.95	0.49
1:B:287:LEU:O	1:B:287:LEU:HD22	2.11	0.49
1:B:341:ARG:O	1:B:344:ASP:HB2	2.12	0.49
1:A:91:ARG:NH2	1:A:362:PRO:HD2	2.28	0.49
1:B:161:ASP:OD1	1:B:208:LYS:HE2	2.12	0.49
1:B:326:SER:OG	1:B:328:HIS:ND1	2.34	0.49
1:B:310:THR:HG22	1:B:311:GLU:N	2.28	0.48
1:B:251:ARG:HB3	1:B:276:TYR:O	2.14	0.48
1:A:203:THR:HG23	1:A:253:LEU:HB2	1.96	0.47
1:B:402:ARG:HB3	1:B:403:PRO:HD3	1.96	0.47
1:B:131:LYS:NZ	1:B:158:GLU:O	2.36	0.47
1:A:203:THR:HB	1:A:250:GLY:O	2.15	0.47
1:A:217:HIS:CD2	1:A:261:PRO:HD3	2.49	0.47
1:A:346:TYR:CG	1:A:406:LEU:HB2	2.50	0.46
1:A:209:ASN:O	1:A:214:LYS:CG	2.63	0.46
1:A:133:ILE:CD1	1:A:439:PRO:HB3	2.45	0.45
1:B:290:ARG:NH2	1:B:337:ASN:HB3	2.31	0.45
1:B:304:ARG:HA	1:B:307:THR:CG2	2.46	0.45
1:A:118:ARG:HG2	1:A:118:ARG:O	2.15	0.45
1:A:133:ILE:HD13	1:A:154:PHE:HZ	1.81	0.45
1:B:203:THR:HG23	1:B:253:LEU:HD12	1.97	0.45
1:A:277:VAL:CG2	1:A:336:LEU:HA	2.46	0.45
1:B:203:THR:CG2	1:B:253:LEU:HB2	2.47	0.45
1:B:303:HIS:HB2	2:B:2039:HOH:O	2.16	0.45
1:B:242:VAL:HG22	1:B:243:GLU:N	2.31	0.45
1:A:197:LYS:HD2	1:A:200:TYR:CG	2.52	0.45
1:A:209:ASN:HD22	1:A:213:VAL:HG21	1.81	0.45
1:A:365:ARG:O	1:A:369:ARG:HG3	2.17	0.44
1:A:151:LEU:O	1:A:155:MET:HG2	2.17	0.44
1:A:415:VAL:HG12	1:A:419:LEU:HB2	1.99	0.44
1:A:242:VAL:HG22	1:A:243:GLU:N	2.33	0.44
1:A:340:GLU:OE2	1:A:341:ARG:HD3	2.18	0.44
1:B:104:SER:H	1:B:107:GLU:CD	2.21	0.44
1:B:332:TRP:HB3	1:B:414:VAL:HB	1.99	0.43
1:B:325:SER:HB2	1:B:418:ARG:HB2	1.99	0.43
1:B:166:GLN:CB	1:B:276:TYR:HB2	2.45	0.43
1:B:192:HIS:HD2	1:B:222:ARG:HD3	1.79	0.43
1:B:90:ILE:HG23	1:B:91:ARG:HG3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:MET:HE2	1:A:218:ALA:CB	2.47	0.43
1:A:341:ARG:O	1:A:344:ASP:HB2	2.19	0.43
1:A:133:ILE:HD11	1:A:439:PRO:CB	2.49	0.43
1:A:242:VAL:HG22	1:A:243:GLU:H	1.83	0.42
1:A:379:ASP:CG	1:A:409:ARG:HH22	2.22	0.42
1:A:290:ARG:NH2	1:A:337:ASN:HB3	2.34	0.42
1:A:395:TRP:HE1	1:A:405:ASN:ND2	2.16	0.42
1:A:214:LYS:HE3	1:A:214:LYS:HB3	1.77	0.42
1:B:135:TRP:O	1:B:165:LEU:HA	2.20	0.42
1:B:208:LYS:HD2	2:B:2023:HOH:O	2.20	0.42
1:B:286:ARG:NH2	2:B:2038:HOH:O	2.52	0.42
1:B:217:HIS:HD2	1:B:258:SER:O	2.02	0.42
1:B:363:GLU:HA	1:B:366:MET:CE	2.49	0.41
1:B:360:PHE:HB2	1:B:408:TRP:CZ3	2.55	0.41
1:B:217:HIS:CD2	1:B:261:PRO:CD	2.92	0.41
1:A:133:ILE:CD1	1:A:439:PRO:CB	2.99	0.41
1:B:287:LEU:N	1:B:288:PRO:HD2	2.35	0.41
1:B:275:THR:HG21	1:B:277:VAL:HG23	2.02	0.41
1:A:203:THR:CG2	1:A:253:LEU:HB2	2.50	0.41
1:B:203:THR:HG23	1:B:253:LEU:HB2	2.03	0.41
1:B:169:LYS:O	1:B:199:GLY:HA2	2.21	0.41
1:B:217:HIS:HD2	1:B:261:PRO:HD3	1.74	0.40
1:A:159:LYS:O	1:A:208:LYS:NZ	2.54	0.40
1:A:192:HIS:CE1	1:A:250:GLY:HA2	2.56	0.40
1:A:134:THR:OG1	1:A:334:GLY:HA2	2.22	0.40
1:A:339:ALA:HB1	1:A:344:ASP:HB3	2.03	0.40
1:B:289:TYR:CD1	1:B:293:SER:HB2	2.56	0.40
1:A:141:ARG:NH1	2:A:2012:HOH:O	2.55	0.40
1:B:363:GLU:HG3	1:B:366:MET:CE	2.51	0.40
1:A:207:MET:CE	1:A:218:ALA:CB	3.00	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	325/467 (70%)	313 (96%)	10 (3%)	2 (1%)	28	46
1	B	325/467 (70%)	313 (96%)	12 (4%)	0	100	100
All	All	650/934 (70%)	626 (96%)	22 (3%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	A	210	SER

### 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	
1	A	284/380 (75%)	258 (91%)	26 (9%)	11	19
1	B	284/380 (75%)	255 (90%)	29 (10%)	8	15
All	All	568/760 (75%)	513 (90%)	55 (10%)	9	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	102	LYS
1	A	106	LYS
1	A	111	ASP
1	A	120	THR
1	A	133	ILE
1	A	162	VAL
1	A	183	VAL
1	A	196	PHE
1	A	203	THR
1	A	214	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	273	VAL
1	A	275	THR
1	A	279	ASN
1	A	282	MET
1	A	307	THR
1	A	310	THR
1	A	340	GLU
1	A	373	GLN
1	A	374	ARG
1	A	383	GLN
1	A	391	VAL
1	A	404	ARG
1	A	406	LEU
1	A	417	SER
1	A	440	PHE
1	B	92	THR
1	B	99	LEU
1	B	133	ILE
1	B	141	ARG
1	B	162	VAL
1	B	176	ASP
1	B	183	VAL
1	B	196	PHE
1	B	197	LYS
1	B	203	THR
1	B	228	SER
1	B	229	GLU
1	B	241	LEU
1	B	251	ARG
1	B	262	ASP
1	B	279	ASN
1	B	280	SER
1	B	286	ARG
1	B	287	LEU
1	B	326	SER
1	B	340	GLU
1	B	373	GLN
1	B	374	ARG
1	B	383	GLN
1	B	400	ASN
1	B	406	LEU
1	B	415	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	440	PHE
1	B	442	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	209	ASN
1	A	217	HIS
1	A	279	ASN
1	A	376	ASN
1	A	387	GLN
1	A	405	ASN
1	A	437	HIS
1	B	192	HIS
1	B	209	ASN
1	B	217	HIS
1	B	279	ASN
1	B	312	ASN
1	B	355	GLN
1	B	376	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 ⓘ

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	333/467 (71%)	0.22	24 (7%) 16 16	29, 41, 72, 81	0
1	B	333/467 (71%)	0.50	39 (11%) 5 4	30, 41, 72, 81	0
All	All	666/934 (71%)	0.36	63 (9%) 9 8	29, 41, 72, 81	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	ALA	6.5
1	B	325	SER	5.9
1	B	400	ASN	5.1
1	B	314	ALA	4.7
1	A	311	GLU	4.3
1	B	326	SER	4.1
1	B	282	MET	3.9
1	B	312	ASN	3.9
1	B	398	ARG	3.8
1	B	262	ASP	3.7
1	B	182	GLY	3.5
1	A	398	ARG	3.5
1	B	403	PRO	3.5
1	A	314	ALA	3.4
1	A	228	SER	3.3
1	B	153	ALA	3.3
1	B	102	LYS	3.3
1	A	313	ALA	3.2
1	B	229	GLU	3.1
1	B	334	GLY	3.1
1	A	312	ASN	3.0
1	A	412	TYR	2.9
1	A	333	ALA	2.9
1	B	156	GLU	2.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	397	GLN	2.7
1	A	325	SER	2.7
1	B	157	ALA	2.6
1	A	403	PRO	2.5
1	B	96	LEU	2.4
1	B	404	ARG	2.4
1	A	282	MET	2.4
1	B	145	LYS	2.4
1	B	399	ILE	2.4
1	A	93	ALA	2.4
1	A	336	LEU	2.3
1	B	151	LEU	2.3
1	B	93	ALA	2.3
1	A	146	LYS	2.3
1	A	100	ASN	2.3
1	B	261	PRO	2.3
1	B	311	GLU	2.3
1	B	152	ARG	2.3
1	A	110	SER	2.3
1	A	90	ILE	2.2
1	B	350	THR	2.2
1	B	336	LEU	2.2
1	B	162	VAL	2.2
1	B	412	TYR	2.2
1	A	92	THR	2.2
1	B	333	ALA	2.2
1	A	133	ILE	2.2
1	B	134	THR	2.2
1	A	334	GLY	2.1
1	A	338	VAL	2.1
1	B	410	LEU	2.1
1	A	102	LYS	2.1
1	B	241	LEU	2.1
1	A	404	ARG	2.1
1	A	406	LEU	2.1
1	B	411	ASP	2.1
1	B	327	PRO	2.0
1	B	275	THR	2.0
1	B	106	LYS	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.