



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:31 pm BST

PDB ID : 3B43  
Title : I-band fragment I65-I70 from titin  
Authors : von Castelmur, E.; Marino, M.; Labeit, D.; Labeit, S.; Mayans, O.  
Deposited on : 2007-10-23  
Resolution : 3.30 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](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

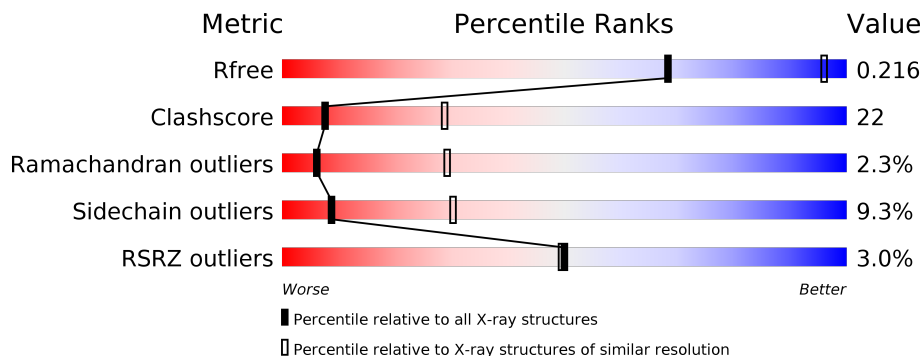
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	570	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4412 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.

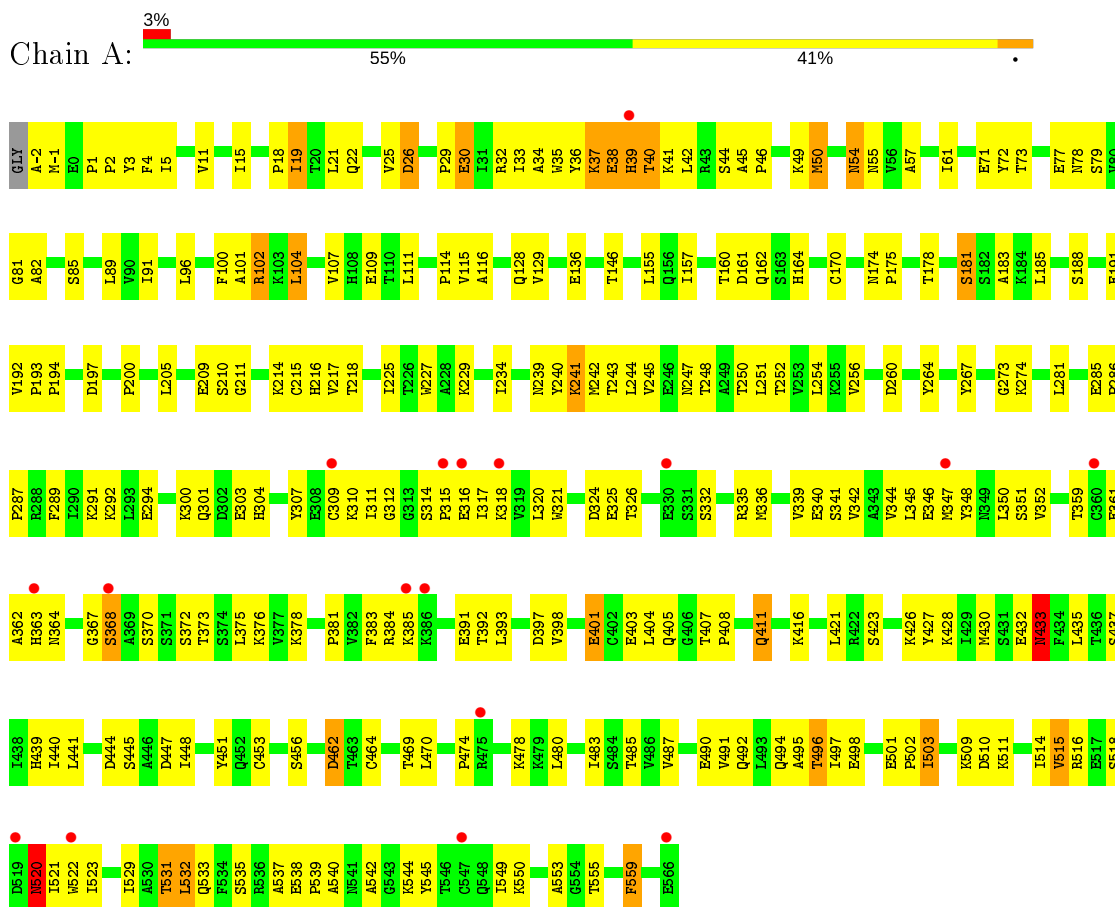
- Molecule 1 is a protein called Titin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	569	4412	2781	745	866	20	0	0	0

### 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 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: Titin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.43Å 141.43Å 166.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.98 – 3.30 16.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (16.98-3.30) 98.6 (16.99-3.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 3.27Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.220 , 0.267 0.221 , 0.216	Depositor DCC
$R_{free}$ test set	741 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.6	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.32	0/4505	0.51	0/6106

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	4412	0	4372	193	0
All	All	4412	0	4372	193	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 22.

All (193) 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:205:LEU:HD11	1:A:211:GLY:HA3	1.61	0.83
1:A:381:PRO:HG2	1:A:456:SER:HA	1.59	0.82
1:A:520:ASN:HD22	1:A:520:ASN:N	1.78	0.81
1:A:45:ALA:HB1	1:A:46:PRO:HD2	1.63	0.80
1:A:428:LYS:HB2	1:A:439:HIS:HB2	1.63	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:HG12	1:A:549:ILE:HG21	1.63	0.79
1:A:33:ILE:HD13	1:A:57:ALA:HB1	1.64	0.79
1:A:101:ALA:O	1:A:102:ARG:HD2	1.84	0.78
1:A:433:ASN:HD22	1:A:433:ASN:H	1.29	0.77
1:A:550:LYS:HG3	1:A:555:THR:HG22	1.68	0.75
1:A:483:ILE:HG21	1:A:491:VAL:HG13	1.71	0.73
1:A:245:VAL:O	1:A:248:THR:HG22	1.89	0.73
1:A:174:ASN:HB2	1:A:175:PRO:HD2	1.72	0.72
1:A:509:LYS:HB2	1:A:514:ILE:HD11	1.71	0.71
1:A:107:VAL:HG11	1:A:115:VAL:CG1	2.22	0.70
1:A:229:LYS:HB2	1:A:234:ILE:HD11	1.74	0.70
1:A:523:ILE:HG22	1:A:532:LEU:HD23	1.75	0.69
1:A:453:CYS:HB3	1:A:464:CYS:HB3	1.75	0.68
1:A:318:LYS:O	1:A:362:ALA:HA	1.94	0.67
1:A:426:LYS:HE3	1:A:441:LEU:O	1.95	0.67
1:A:146:THR:HG22	1:A:155:LEU:HD23	1.75	0.67
1:A:161:ASP:HB3	1:A:164:HIS:CD2	2.31	0.66
1:A:33:ILE:HD12	1:A:35:TRP:NE1	2.12	0.65
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.62	0.65
1:A:494:GLN:HE21	1:A:531:THR:CG2	2.10	0.64
1:A:416:LYS:HD2	1:A:451:TYR:CZ	2.34	0.63
1:A:311:ILE:HD13	1:A:362:ALA:HB2	1.80	0.62
1:A:497:ILE:CG1	1:A:549:ILE:HG21	2.30	0.62
1:A:324:ASP:O	1:A:325:GLU:HB2	2.00	0.61
1:A:515:VAL:HG12	1:A:516:ARG:H	1.66	0.61
1:A:287:PRO:HA	1:A:312:GLY:O	2.01	0.60
1:A:335:ARG:HG3	1:A:348:TYR:HE2	1.67	0.60
1:A:115:VAL:HG23	1:A:160:THR:HG21	1.84	0.60
1:A:378:LYS:HG2	1:A:407:THR:HG21	1.83	0.59
1:A:104:LEU:O	1:A:183:ALA:HB2	2.02	0.59
1:A:291:LYS:H	1:A:310:LYS:HB3	1.66	0.59
1:A:115:VAL:CG2	1:A:160:THR:HG21	2.32	0.59
1:A:229:LYS:HG3	1:A:264:TYR:CZ	2.38	0.58
1:A:114:PRO:HA	1:A:157:ILE:O	2.04	0.57
1:A:544:LYS:HE2	1:A:559:PHE:CE2	2.39	0.57
1:A:241:LYS:HG3	1:A:252:THR:HB	1.86	0.57
1:A:520:ASN:HA	1:A:535:SER:OG	2.05	0.57
1:A:335:ARG:O	1:A:336:MET:HG3	2.05	0.56
1:A:39:HIS:O	1:A:39:HIS:CG	2.59	0.56
1:A:544:LYS:HE2	1:A:559:PHE:CD2	2.41	0.56
1:A:286:PRO:HB3	1:A:367:GLY:HA3	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:O	1:A:39:HIS:N	2.39	0.56
1:A:33:ILE:HD12	1:A:35:TRP:HE1	1.71	0.56
1:A:433:ASN:HD22	1:A:433:ASN:N	1.99	0.56
1:A:516:ARG:HH12	1:A:522:TRP:HE3	1.54	0.56
1:A:29:PRO:O	1:A:30:GLU:HB2	2.05	0.56
1:A:240:TYR:HB3	1:A:251:LEU:HD21	1.89	0.55
1:A:347:MET:HB3	1:A:350:LEU:HD21	1.88	0.55
1:A:497:ILE:HG12	1:A:549:ILE:CG2	2.34	0.55
1:A:494:GLN:HE21	1:A:531:THR:HG22	1.72	0.55
1:A:197:ASP:OD2	1:A:218:THR:HG23	2.08	0.54
1:A:385:LYS:HB2	1:A:403:GLU:HG3	1.89	0.54
1:A:287:PRO:HD3	1:A:364:ASN:CG	2.28	0.54
1:A:3:TYR:CZ	1:A:26:ASP:HB3	2.42	0.54
1:A:509:LYS:HG2	1:A:544:LYS:O	2.09	0.53
1:A:104:LEU:HB2	1:A:181:SER:HB3	1.90	0.53
1:A:38:GLU:HG3	1:A:71:GLU:OE2	2.09	0.53
1:A:487:VAL:HG13	1:A:538:GLU:HA	1.91	0.53
1:A:161:ASP:N	1:A:164:HIS:HD2	2.07	0.53
1:A:2:PRO:HD3	1:A:78:ASN:CG	2.29	0.52
1:A:30:GLU:OE1	1:A:30:GLU:HA	2.10	0.52
1:A:320:LEU:HD12	1:A:320:LEU:N	2.25	0.52
1:A:342:VAL:HG12	1:A:344:VAL:HG23	1.92	0.52
1:A:146:THR:CG2	1:A:155:LEU:HD23	2.40	0.52
1:A:501:GLU:O	1:A:503:ILE:HG12	2.10	0.52
1:A:45:ALA:HB1	1:A:46:PRO:CD	2.39	0.51
1:A:197:ASP:OD2	1:A:216:HIS:CD2	2.64	0.51
1:A:4:PHE:CE2	1:A:85:SER:HB2	2.45	0.51
1:A:393:LEU:CD2	1:A:553:ALA:HA	2.40	0.51
1:A:520:ASN:N	1:A:520:ASN:ND2	2.51	0.51
1:A:495:ALA:O	1:A:529:ILE:HG13	2.09	0.51
1:A:393:LEU:HD23	1:A:553:ALA:HA	1.94	0.50
1:A:89:LEU:HD23	1:A:89:LEU:C	2.31	0.50
1:A:164:HIS:O	1:A:185:LEU:HD23	2.10	0.50
1:A:550:LYS:HG3	1:A:555:THR:CG2	2.39	0.50
1:A:107:VAL:HG11	1:A:115:VAL:HG11	1.92	0.50
1:A:210:SER:HB3	1:A:254:LEU:O	2.12	0.50
1:A:383:PHE:CD2	1:A:462:ASP:HB3	2.47	0.50
1:A:260:ASP:O	1:A:281:LEU:HD23	2.11	0.50
1:A:320:LEU:HD11	1:A:363:HIS:HE1	1.75	0.50
1:A:320:LEU:HD11	1:A:363:HIS:CE1	2.47	0.49
1:A:77:GLU:HG2	1:A:82:ALA:HB2	1.93	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG22	1:A:61:ILE:HB	1.94	0.49
1:A:229:LYS:H	1:A:234:ILE:HG13	1.77	0.49
1:A:397:ASP:OD2	1:A:441:LEU:HD22	2.13	0.48
1:A:136:GLU:HA	1:A:136:GLU:OE2	2.13	0.48
1:A:440:ILE:HD12	1:A:440:ILE:H	1.79	0.48
1:A:392:THR:O	1:A:470:LEU:HD12	2.13	0.48
1:A:516:ARG:HD2	1:A:523:ILE:HG12	1.93	0.48
1:A:559:PHE:C	1:A:559:PHE:CD1	2.87	0.48
1:A:335:ARG:HG3	1:A:348:TYR:CE2	2.46	0.48
1:A:485:THR:HG21	1:A:491:VAL:HG22	1.96	0.48
1:A:335:ARG:O	1:A:345:LEU:HD12	2.13	0.48
1:A:440:ILE:HD12	1:A:440:ILE:N	2.28	0.47
1:A:336:MET:HA	1:A:344:VAL:O	2.14	0.47
1:A:303:GLU:HB3	1:A:304:HIS:H	1.53	0.47
1:A:33:ILE:CD1	1:A:35:TRP:HE1	2.26	0.47
1:A:38:GLU:C	1:A:40:THR:H	2.18	0.47
1:A:516:ARG:O	1:A:516:ARG:HG3	2.14	0.47
1:A:311:ILE:HD13	1:A:362:ALA:CB	2.44	0.47
1:A:540:ALA:C	1:A:542:ALA:H	2.18	0.47
1:A:146:THR:HG22	1:A:155:LEU:CD2	2.44	0.47
1:A:5:ILE:HD11	1:A:26:ASP:HB2	1.96	0.47
1:A:391:GLU:HB3	1:A:469:THR:OG1	2.15	0.47
1:A:200:PRO:HD3	1:A:215:CYS:HB3	1.96	0.46
1:A:251:LEU:HD13	1:A:251:LEU:C	2.35	0.46
1:A:361:GLU:OE2	1:A:370:SER:HB3	2.15	0.46
1:A:310:LYS:HA	1:A:341:SER:O	2.15	0.46
1:A:273:GLY:O	1:A:274:LYS:HG3	2.15	0.46
1:A:340:GLU:O	1:A:341:SER:HB2	2.15	0.46
1:A:401:GLU:CB	1:A:437:SER:HB3	2.45	0.46
1:A:211:GLY:O	1:A:252:THR:HG23	2.16	0.46
1:A:50:MET:HB3	1:A:50:MET:HE2	1.73	0.46
1:A:359:THR:HG23	1:A:372:SER:OG	2.15	0.46
1:A:321:TRP:NE1	1:A:336:MET:HG2	2.30	0.46
1:A:391:GLU:HA	1:A:469:THR:O	2.16	0.46
1:A:214:LYS:HB2	1:A:214:LYS:HE2	1.73	0.45
1:A:538:GLU:HB2	1:A:539:PRO:HD2	1.99	0.45
1:A:248:THR:HG23	1:A:248:THR:O	2.16	0.45
1:A:478:LYS:HD2	1:A:496:THR:OG1	2.16	0.45
1:A:289:PHE:HB3	1:A:292:LYS:HG2	1.98	0.45
1:A:21:LEU:HD12	1:A:21:LEU:N	2.32	0.45
1:A:239:ASN:ND2	1:A:260:ASP:OD2	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:O	1:A:348:TYR:HD2	2.00	0.45
1:A:301:GLN:HG3	1:A:351:SER:HA	1.98	0.45
1:A:307:TYR:CE1	1:A:373:THR:HG21	2.52	0.45
1:A:426:LYS:HE2	1:A:447:ASP:OD2	2.17	0.45
1:A:383:PHE:CE2	1:A:464:CYS:HB2	2.52	0.44
1:A:375:LEU:HG	1:A:376:LYS:N	2.32	0.44
1:A:42:LEU:HA	1:A:42:LEU:HD13	1.80	0.44
1:A:516:ARG:NH1	1:A:522:TRP:CE3	2.85	0.44
1:A:33:ILE:O	1:A:33:ILE:HG13	2.18	0.44
1:A:375:LEU:HG	1:A:376:LYS:H	1.82	0.44
1:A:432:GLU:O	1:A:433:ASN:C	2.56	0.44
1:A:433:ASN:ND2	1:A:433:ASN:H	2.06	0.44
1:A:478:LYS:HB2	1:A:496:THR:OG1	2.17	0.44
1:A:501:GLU:H	1:A:501:GLU:HG2	1.59	0.44
1:A:539:PRO:O	1:A:540:ALA:HB3	2.18	0.44
1:A:19:ILE:HA	1:A:19:ILE:HD12	1.84	0.44
1:A:242:MET:HG2	1:A:251:LEU:HD23	1.99	0.44
1:A:520:ASN:ND2	1:A:521:ILE:HD12	2.33	0.44
1:A:205:LEU:HB2	1:A:281:LEU:HD11	2.00	0.44
1:A:36:TYR:HB2	1:A:73:THR:HB	2.00	0.44
1:A:509:LYS:HG3	1:A:545:TYR:CE1	2.53	0.43
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.79	0.43
1:A:225:ILE:HA	1:A:267:TYR:O	2.18	0.43
1:A:510:ASP:O	1:A:511:LYS:HB2	2.18	0.43
1:A:518:SER:HG	1:A:522:TRP:HE1	1.66	0.43
1:A:383:PHE:CD2	1:A:464:CYS:HB2	2.54	0.43
1:A:-2:ALA:HA	1:A:-1:MET:HA	1.59	0.43
1:A:115:VAL:HG12	1:A:116:ALA:N	2.34	0.43
1:A:339:VAL:HG23	1:A:339:VAL:O	2.19	0.43
1:A:516:ARG:NH1	1:A:522:TRP:HE3	2.15	0.43
1:A:537:ALA:O	1:A:538:GLU:HB3	2.19	0.43
1:A:314:SER:HB2	1:A:364:ASN:HD22	1.84	0.42
1:A:474:PRO:HB2	1:A:549:ILE:HG13	2.00	0.42
1:A:128:GLN:HG3	1:A:129:VAL:N	2.32	0.42
1:A:18:PRO:HA	1:A:61:ILE:O	2.18	0.42
1:A:37:LYS:HE2	1:A:72:TYR:CE1	2.55	0.42
1:A:107:VAL:HG11	1:A:115:VAL:HG13	1.98	0.42
1:A:100:PHE:HZ	1:A:170:CYS:O	2.02	0.42
1:A:401:GLU:HB2	1:A:437:SER:HB3	2.01	0.42
1:A:54:ASN:HB3	1:A:55:ASN:H	1.60	0.42
1:A:242:MET:CG	1:A:251:LEU:HD23	2.50	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PRO:HB3	1:A:81:GLY:HA3	2.02	0.42
1:A:445:SER:HA	1:A:448:ILE:HG12	2.02	0.41
1:A:245:VAL:HG23	1:A:245:VAL:O	2.20	0.41
1:A:314:SER:HB2	1:A:364:ASN:ND2	2.35	0.41
1:A:404:LEU:HD12	1:A:405:GLN:H	1.85	0.41
1:A:34:ALA:HB1	1:A:41:LYS:HE3	2.03	0.41
1:A:492:GLN:HE21	1:A:533:GLN:HG3	1.84	0.41
1:A:501:GLU:N	1:A:502:PRO:CD	2.83	0.41
1:A:497:ILE:CG2	1:A:498:GLU:N	2.83	0.41
1:A:227:TRP:HD1	1:A:242:MET:CE	2.33	0.41
1:A:227:TRP:HD1	1:A:242:MET:HE2	1.86	0.41
1:A:315:PRO:O	1:A:316:GLU:HB2	2.20	0.41
1:A:217:VAL:O	1:A:247:ASN:HB3	2.20	0.41
1:A:421:LEU:HD22	1:A:427:TYR:CE2	2.56	0.41
1:A:192:VAL:HA	1:A:193:PRO:HD2	1.94	0.41
1:A:300:LYS:HG2	1:A:301:GLN:O	2.21	0.40
1:A:2:PRO:HD3	1:A:78:ASN:ND2	2.36	0.40
1:A:91:ILE:HA	1:A:91:ILE:HD13	1.79	0.40
1:A:363:HIS:CB	1:A:368:SER:HB3	2.52	0.40
1:A:494:GLN:HE21	1:A:531:THR:HG21	1.83	0.40
1:A:335:ARG:HB2	1:A:346:GLU:HB3	2.03	0.40
1:A:490:GLU:HG2	1:A:535:SER:O	2.22	0.40
1:A:480:LEU:HD23	1:A:494:GLN:O	2.21	0.40
1:A:407:THR:HA	1:A:408:PRO:HD2	1.80	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	567/570 (100%)	502 (88%)	52 (9%)	13 (2%)	<b>6</b> 29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	384	ARG
1	A	520	ASN
1	A	39	HIS
1	A	423	SER
1	A	433	ASN
1	A	368	SER
1	A	30	GLU
1	A	209	GLU
1	A	515	VAL
1	A	54	ASN
1	A	79	SER
1	A	256	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
1	A	492/492 (100%)	446 (91%)	46 (9%)	9 30

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	15	ILE
1	A	19	ILE
1	A	22	GLN
1	A	25	VAL
1	A	26	ASP
1	A	32	ARG
1	A	37	LYS
1	A	40	THR
1	A	44	SER
1	A	49	LYS
1	A	50	MET

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	96	LEU
1	A	102	ARG
1	A	104	LEU
1	A	109	GLU
1	A	111	LEU
1	A	162	GLN
1	A	178	THR
1	A	181	SER
1	A	188	SER
1	A	191	GLU
1	A	241	LYS
1	A	243	THR
1	A	244	LEU
1	A	250	THR
1	A	285	GLU
1	A	294	GLU
1	A	309	CYS
1	A	317	ILE
1	A	326	THR
1	A	352	VAL
1	A	398	VAL
1	A	401	GLU
1	A	411	GLN
1	A	430	MET
1	A	433	ASN
1	A	435	LEU
1	A	444	ASP
1	A	462	ASP
1	A	496	THR
1	A	503	ILE
1	A	520	ASN
1	A	531	THR
1	A	532	LEU
1	A	559	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	55	ASN
1	A	62	ASN
1	A	151	ASN
1	A	164	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	216	HIS
1	A	231	ASN
1	A	363	HIS
1	A	411	GLN
1	A	433	ASN
1	A	492	GLN
1	A	494	GLN
1	A	520	ASN
1	A	541	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 [i](#)

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

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	569/570 (99%)	-0.09	17 (2%) 50 49	49, 116, 182, 215	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	GLU	4.1
1	A	519	ASP	3.8
1	A	315	PRO	3.5
1	A	522	TRP	2.8
1	A	386	LYS	2.7
1	A	363	HIS	2.7
1	A	39	HIS	2.5
1	A	318	LYS	2.4
1	A	368	SER	2.3
1	A	360	CYS	2.2
1	A	309	CYS	2.1
1	A	547	CYS	2.1
1	A	385	LYS	2.1
1	A	330	GLU	2.0
1	A	347	MET	2.0
1	A	316	GLU	2.0
1	A	475	ARG	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.