Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:52 PM GMT

PDB ID	:	1YUW
Title	:	crystal structure of bovine hsc70(aa1-554)E213A/D214A mutant
Authors	:	Jiang, J.; Lafer, E.M.; Prasad, K.; Sousa, R.
Deposited on	:	2005-02-14
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

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 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.
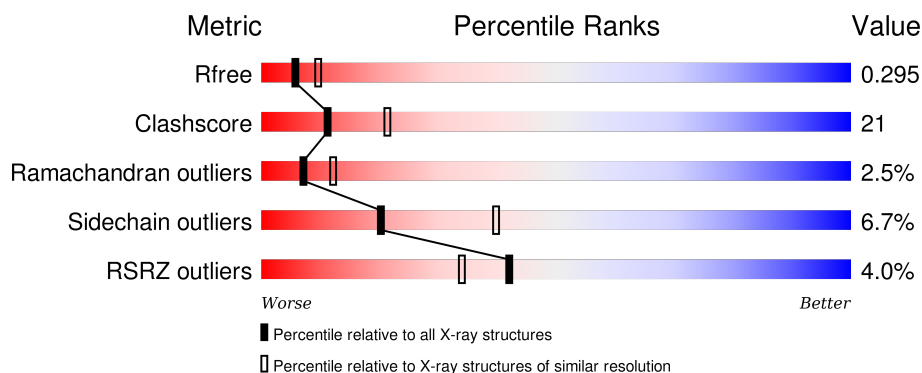
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	554	4% (red) / 62% (green) / 32% (yellow) / 5% (orange)

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4403 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 Heat shock cognate 71 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4282	2680	744	845	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	GLU	ENGINEERED	UNP P19120
A	214	ALA	ASP	ENGINEERED	UNP P19120

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	121	121	121	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 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.

• Molecule 1: Heat shock cognate 71 kDa protein
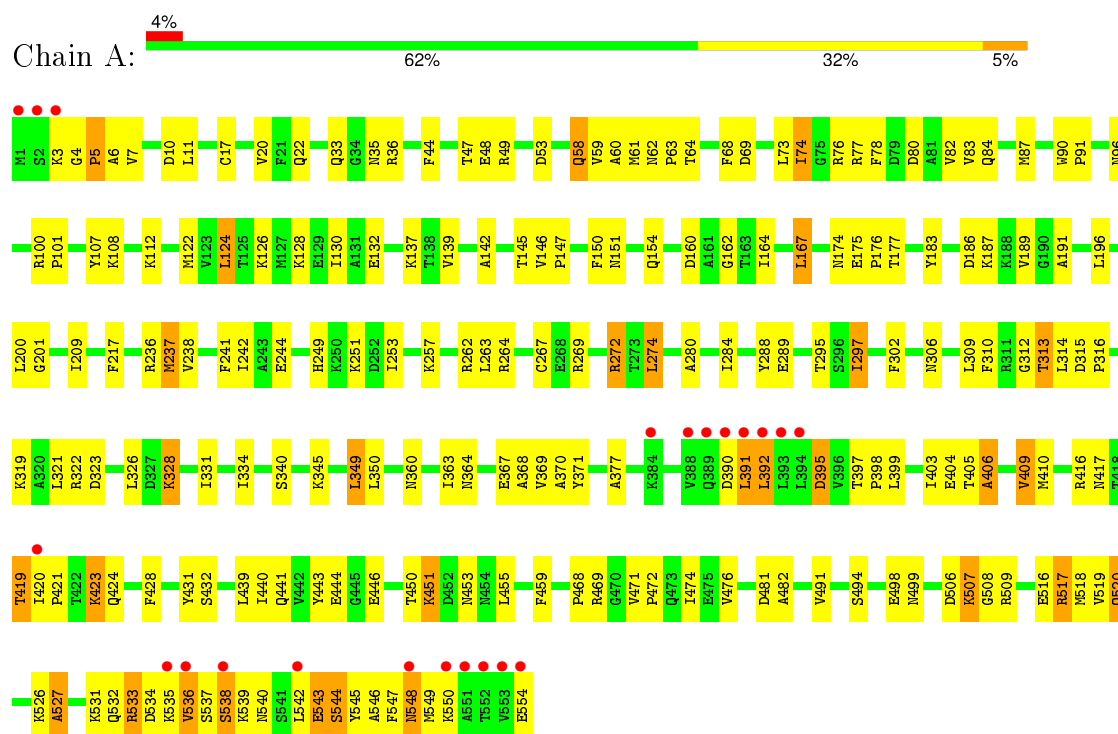
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.69Å 50.14Å 87.16Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 34.63 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 92.7 (34.63-2.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.18 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.297 0.224 , 0.295	Depositor DCC
R_{free} test set	1640 reflections (9.93%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 17674 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4403	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/4343	0.62	0/5864

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	4282	0	4316	178	0
2	A	121	0	0	10	0
All	All	4403	0	4316	178	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 (178) 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:420:ILE:HG23	1:A:421:PRO:HD3	1.15	1.14
1:A:272:ARG:HB3	1:A:272:ARG:HH11	1.27	0.97
1:A:536:VAL:HG12	1:A:537:SER:H	1.39	0.87
1:A:420:ILE:HG23	1:A:421:PRO:CD	2.04	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ILE:CG2	1:A:421:PRO:HD3	2.04	0.85
1:A:297:ILE:H	1:A:297:ILE:HD12	1.44	0.82
1:A:310:PHE:O	1:A:313:THR:HB	1.78	0.82
1:A:272:ARG:HB3	1:A:272:ARG:NH1	1.95	0.81
1:A:315:ASP:HB2	1:A:316:PRO:HD3	1.63	0.78
1:A:520:GLN:HE21	1:A:520:GLN:HA	1.49	0.78
1:A:151:ASN:H	1:A:154:GLN:HE21	1.33	0.76
1:A:200:LEU:HG	1:A:340:SER:HB2	1.67	0.76
1:A:406:ALA:HA	1:A:542:LEU:HG	1.67	0.76
1:A:272:ARG:CB	1:A:272:ARG:HH11	1.99	0.75
1:A:451:LYS:HD2	1:A:451:LYS:N	2.03	0.74
1:A:532:GLN:HE21	1:A:535:LYS:HB2	1.53	0.73
1:A:516:GLU:O	1:A:520:GLN:HG2	1.89	0.71
1:A:264:ARG:NH1	1:A:264:ARG:HB2	2.05	0.71
1:A:264:ARG:HH11	1:A:264:ARG:HB2	1.56	0.70
1:A:439:LEU:HB2	1:A:544:SER:HA	1.73	0.70
1:A:391:LEU:HG	1:A:392:LEU:HD23	1.72	0.70
1:A:543:GLU:O	1:A:544:SER:HB2	1.92	0.69
1:A:313:THR:HG22	1:A:314:LEU:HD12	1.77	0.67
1:A:151:ASN:H	1:A:154:GLN:NE2	1.94	0.65
1:A:236:ARG:HG3	1:A:306:ASN:OD1	1.96	0.65
1:A:537:SER:O	1:A:538:SER:HB3	1.97	0.65
1:A:83:VAL:O	1:A:87:MET:HG3	1.96	0.65
1:A:542:LEU:HD22	1:A:545:TYR:CZ	2.32	0.65
1:A:58:GLN:HE22	1:A:62:ASN:HB3	1.63	0.64
1:A:474:ILE:N	1:A:474:ILE:HD12	2.14	0.63
1:A:334:ILE:HG21	1:A:350:LEU:HD11	1.80	0.63
1:A:4:GLY:N	1:A:137:LYS:HE2	2.14	0.63
1:A:200:LEU:HG	1:A:340:SER:CB	2.27	0.63
1:A:546:ALA:C	1:A:548:ASN:H	2.03	0.61
1:A:532:GLN:NE2	1:A:535:LYS:HB2	2.15	0.61
1:A:542:LEU:O	1:A:544:SER:N	2.27	0.61
1:A:507:LYS:O	1:A:509:ARG:N	2.33	0.60
1:A:174:ASN:HB3	1:A:176:PRO:HD2	1.82	0.60
1:A:5:PRO:HD3	1:A:137:LYS:CE	2.31	0.60
1:A:516:GLU:HA	1:A:519:VAL:HG22	1.85	0.59
1:A:536:VAL:HG12	1:A:537:SER:N	2.13	0.59
1:A:469:ARG:C	1:A:469:ARG:HD2	2.23	0.59
1:A:126:LYS:O	1:A:130:ILE:HG13	2.03	0.58
1:A:274:LEU:HD13	1:A:280:ALA:HB2	1.85	0.58
1:A:405:THR:OG1	1:A:409:VAL:HG22	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:HD3	1:A:137:LYS:HE2	1.86	0.58
1:A:494:SER:HB3	2:A:640:HOH:O	2.03	0.57
1:A:68:PHE:O	1:A:69:ASP:HB2	2.04	0.57
1:A:517:ARG:HH11	1:A:517:ARG:HG3	1.69	0.57
1:A:237:MET:HG2	1:A:267:CYS:SG	2.45	0.56
1:A:313:THR:HG22	1:A:314:LEU:CD1	2.35	0.56
1:A:406:ALA:HA	1:A:542:LEU:CG	2.35	0.56
1:A:10:ASP:HB2	1:A:369:VAL:HG12	1.88	0.56
1:A:403:ILE:HG23	2:A:559:HOH:O	2.05	0.56
1:A:128:LYS:O	1:A:132:GLU:HG3	2.06	0.55
1:A:4:GLY:H	1:A:137:LYS:HE2	1.71	0.55
1:A:516:GLU:O	1:A:519:VAL:HG22	2.07	0.55
1:A:548:ASN:ND2	1:A:548:ASN:O	2.39	0.55
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.88	0.55
1:A:549:MET:HG3	1:A:550:LYS:N	2.21	0.54
1:A:423:LYS:HG3	1:A:423:LYS:O	2.07	0.54
1:A:62:ASN:N	1:A:63:PRO:HD3	2.21	0.54
1:A:61:MET:C	1:A:63:PRO:HD3	2.29	0.54
1:A:451:LYS:H	1:A:451:LYS:HD2	1.70	0.53
1:A:3:LYS:HG3	1:A:3:LYS:O	2.08	0.53
1:A:368:ALA:O	1:A:371:TYR:HB3	2.08	0.53
1:A:312:GLY:HA3	2:A:603:HOH:O	2.08	0.53
1:A:6:ALA:O	1:A:20:VAL:HG23	2.08	0.53
1:A:403:ILE:HD12	1:A:476:VAL:HG11	1.91	0.52
1:A:506:ASP:O	1:A:507:LYS:HB3	2.08	0.52
1:A:160:ASP:O	1:A:164:ILE:HG13	2.09	0.52
1:A:237:MET:HE2	1:A:302:PHE:HE1	1.75	0.52
1:A:444:GLU:O	1:A:453:ASN:HB3	2.10	0.52
1:A:237:MET:HE2	1:A:302:PHE:CE1	2.45	0.52
1:A:249:HIS:O	1:A:251:LYS:HG2	2.10	0.52
1:A:151:ASN:OD1	1:A:154:GLN:HG3	2.10	0.51
1:A:538:SER:OG	1:A:539:LYS:N	2.43	0.51
1:A:542:LEU:HD22	1:A:545:TYR:CE1	2.45	0.51
1:A:5:PRO:HD3	1:A:137:LYS:NZ	2.26	0.51
1:A:47:THR:O	1:A:48:GLU:HB3	2.10	0.51
1:A:241:PHE:HZ	1:A:297:ILE:HG13	1.76	0.51
1:A:431:TYR:O	1:A:469:ARG:HG3	2.11	0.51
1:A:80:ASP:O	1:A:80:ASP:OD1	2.29	0.51
1:A:6:ALA:HB1	1:A:377:ALA:HB1	1.93	0.51
1:A:191:ALA:HA	2:A:648:HOH:O	2.10	0.51
1:A:506:ASP:O	1:A:507:LYS:CB	2.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HG3	1:A:36:ARG:HH11	1.76	0.50
1:A:80:ASP:O	1:A:82:VAL:N	2.41	0.50
1:A:416:ARG:O	1:A:417:ASN:HB2	2.10	0.50
1:A:419:THR:HG22	1:A:420:ILE:N	2.27	0.50
1:A:404:GLU:HB2	1:A:450:THR:HG21	1.93	0.50
1:A:542:LEU:C	1:A:544:SER:H	2.10	0.49
1:A:416:ARG:HD2	1:A:446:GLU:CD	2.31	0.49
1:A:132:GLU:HG2	1:A:139:VAL:HG23	1.93	0.49
1:A:4:GLY:CA	1:A:137:LYS:HE2	2.42	0.49
1:A:244:GLU:OE2	1:A:295:THR:HG21	2.12	0.49
1:A:112:LYS:HE2	2:A:595:HOH:O	2.12	0.49
1:A:4:GLY:HA2	1:A:137:LYS:HE2	1.95	0.49
1:A:532:GLN:C	1:A:534:ASP:H	2.16	0.49
1:A:183:TYR:CE1	1:A:360:ASN:HB3	2.48	0.49
1:A:321:LEU:HD21	1:A:328:LYS:HA	1.95	0.49
1:A:17:CYS:HB3	1:A:370:ALA:HB2	1.95	0.49
1:A:107:TYR:CZ	1:A:108:LYS:HE3	2.48	0.49
1:A:11:LEU:HD13	1:A:124:LEU:CD1	2.43	0.48
1:A:90:TRP:HB2	2:A:668:HOH:O	2.13	0.48
1:A:517:ARG:HH21	1:A:518:MET:HG3	1.78	0.48
1:A:468:PRO:O	1:A:471:VAL:HG23	2.14	0.48
1:A:288:TYR:CD1	1:A:289:GLU:HG3	2.50	0.47
1:A:177:THR:HG23	1:A:217:PHE:CD1	2.50	0.47
1:A:399:LEU:HD11	1:A:518:MET:CE	2.45	0.47
1:A:78:PHE:CG	1:A:96:ASN:HB2	2.51	0.46
1:A:186:ASP:OD2	1:A:187:LYS:HG3	2.15	0.46
1:A:78:PHE:HA	1:A:101:PRO:HG3	1.98	0.46
1:A:36:ARG:HG3	1:A:36:ARG:NH1	2.30	0.46
1:A:546:ALA:C	1:A:548:ASN:N	2.70	0.45
1:A:257:LYS:HD3	1:A:257:LYS:N	2.31	0.45
1:A:319:LYS:HE2	1:A:323:ASP:OD2	2.17	0.45
1:A:175:GLU:N	1:A:176:PRO:CD	2.80	0.45
1:A:238:VAL:O	1:A:242:ILE:HG13	2.17	0.45
1:A:546:ALA:O	1:A:548:ASN:N	2.49	0.45
1:A:11:LEU:HD13	1:A:124:LEU:HD13	1.99	0.45
1:A:186:ASP:HB3	1:A:217:PHE:CZ	2.52	0.45
1:A:44:PHE:O	1:A:62:ASN:ND2	2.45	0.44
1:A:73:LEU:HD21	1:A:90:TRP:CH2	2.52	0.44
1:A:196:LEU:HD23	1:A:196:LEU:C	2.38	0.44
1:A:146:VAL:HG13	1:A:147:PRO:CD	2.48	0.44
1:A:78:PHE:O	1:A:84:GLN:NE2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.81	0.44
1:A:441:GLN:HG2	2:A:559:HOH:O	2.18	0.44
1:A:288:TYR:CE1	1:A:289:GLU:HG3	2.53	0.44
1:A:238:VAL:CG2	1:A:264:ARG:HA	2.48	0.44
1:A:58:GLN:NE2	1:A:62:ASN:HB3	2.30	0.44
1:A:280:ALA:HB3	1:A:297:ILE:CD1	2.47	0.43
1:A:443:TYR:CZ	1:A:455:LEU:HD13	2.53	0.43
1:A:64:THR:HG23	2:A:581:HOH:O	2.18	0.43
1:A:10:ASP:HA	1:A:145:THR:OG1	2.18	0.43
1:A:322:ARG:HG3	1:A:322:ARG:HH11	1.82	0.43
1:A:264:ARG:CB	1:A:264:ARG:HH11	2.27	0.43
1:A:520:GLN:NE2	1:A:520:GLN:HA	2.26	0.43
1:A:196:LEU:HD12	1:A:209:ILE:HD11	1.99	0.43
1:A:49:ARG:NE	1:A:122:MET:CE	2.82	0.43
1:A:395:ASP:HB2	1:A:420:ILE:HG21	2.00	0.43
1:A:420:ILE:HD11	1:A:482:ALA:O	2.19	0.42
1:A:532:GLN:HE21	1:A:535:LYS:CB	2.26	0.42
1:A:74:ILE:HD12	1:A:74:ILE:HA	1.82	0.42
1:A:405:THR:O	1:A:406:ALA:C	2.57	0.42
1:A:526:LYS:O	1:A:527:ALA:HB2	2.19	0.42
1:A:262:ARG:NH2	1:A:284:ILE:HG23	2.34	0.42
1:A:90:TRP:HA	1:A:91:PRO:HD3	1.86	0.42
1:A:319:LYS:HG2	1:A:323:ASP:OD2	2.20	0.42
1:A:367:GLU:O	1:A:368:ALA:C	2.58	0.42
1:A:162:GLY:O	1:A:167:LEU:HB2	2.20	0.42
1:A:534:ASP:C	1:A:534:ASP:OD2	2.59	0.42
1:A:471:VAL:HB	1:A:472:PRO:HD3	2.02	0.42
1:A:431:TYR:O	1:A:469:ARG:CG	2.68	0.41
1:A:428:PHE:CD2	1:A:539:LYS:HB3	2.55	0.41
1:A:406:ALA:HA	1:A:542:LEU:CD2	2.50	0.41
1:A:531:LYS:C	1:A:533:ARG:N	2.73	0.41
1:A:535:LYS:HD2	1:A:535:LYS:HA	1.83	0.41
1:A:546:ALA:HB1	2:A:570:HOH:O	2.19	0.41
1:A:253:ILE:HD11	1:A:263:LEU:HD22	2.03	0.41
1:A:35:ASN:ND2	1:A:53:ASP:OD2	2.52	0.41
1:A:59:VAL:HG13	1:A:60:ALA:N	2.35	0.41
1:A:345:LYS:HE3	1:A:349:LEU:HD11	2.03	0.41
1:A:363:ILE:O	1:A:364:ASN:C	2.58	0.41
1:A:419:THR:CG2	1:A:420:ILE:N	2.84	0.41
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.78	0.41
1:A:440:ILE:HG21	1:A:459:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HA	1:A:398:PRO:HD3	1.91	0.41
1:A:49:ARG:NE	1:A:122:MET:HE1	2.36	0.41
1:A:201:GLY:HA3	2:A:622:HOH:O	2.20	0.40
1:A:491:VAL:HG22	1:A:498:GLU:HB3	2.02	0.40
1:A:7:VAL:O	1:A:142:ALA:HA	2.21	0.40
1:A:269:ARG:HB2	1:A:269:ARG:CZ	2.52	0.40
1:A:77:ARG:NH1	1:A:77:ARG:HB3	2.36	0.40
1:A:481:ASP:C	1:A:481:ASP:OD1	2.60	0.40
1:A:146:VAL:HG13	1:A:150:PHE:CD2	2.56	0.40
1:A:321:LEU:HD11	1:A:331:ILE:HD11	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	552/554 (100%)	489 (89%)	49 (9%)	14 (2%)	7	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	LYS
1	A	527	ALA
1	A	543	GLU
1	A	391	LEU
1	A	508	GLY
1	A	538	SER
1	A	547	PHE
1	A	5	PRO
1	A	406	ALA
1	A	189	VAL
1	A	419	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	536	VAL
1	A	544	SER
1	A	74	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	466/466 (100%)	435 (93%)	31 (7%)	20 40

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	33	GLN
1	A	58	GLN
1	A	100	ARG
1	A	124	LEU
1	A	167	LEU
1	A	237	MET
1	A	272	ARG
1	A	274	LEU
1	A	297	ILE
1	A	309	LEU
1	A	313	THR
1	A	326	LEU
1	A	328	LYS
1	A	349	LEU
1	A	390	ASP
1	A	392	LEU
1	A	395	ASP
1	A	409	VAL
1	A	410	MET
1	A	423	LYS
1	A	424	GLN
1	A	432	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	LYS
1	A	499	ASN
1	A	517	ARG
1	A	520	GLN
1	A	533	ARG
1	A	540	ASN
1	A	548	ASN
1	A	554	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	141	ASN
1	A	154	GLN
1	A	156	GLN
1	A	227	HIS
1	A	240	HIS
1	A	279	GLN
1	A	454	ASN
1	A	499	ASN
1	A	520	GLN
1	A	532	GLN
1	A	548	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, 95th 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^2)	Q<0.9
1	A	554/554 (100%)	-0.28	22 (3%)	42	34	8, 27, 86, 148	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	VAL	9.1
1	A	389	GLN	6.8
1	A	554	GLU	5.3
1	A	388	VAL	5.2
1	A	3	LYS	5.2
1	A	390	ASP	4.8
1	A	552	THR	4.3
1	A	393	LEU	3.8
1	A	1	MET	3.7
1	A	2	SER	3.4
1	A	392	LEU	3.3
1	A	391	LEU	3.3
1	A	548	ASN	2.9
1	A	551	ALA	2.6
1	A	550	LYS	2.6
1	A	420	ILE	2.5
1	A	536	VAL	2.5
1	A	538	SER	2.4
1	A	384	LYS	2.2
1	A	535	LYS	2.2
1	A	394	LEU	2.1
1	A	542	LEU	2.1

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.