Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:27 AM GMT

PDB ID	:	2QUQ
Title	:	Crystal Structure of the Essential Inner Kinetochore Protein Cep3p
Authors	:	Bellizzi III, J.J.; Harrison, S.C.
Deposited on	:	2007-08-06
Resolution	:	2.80 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

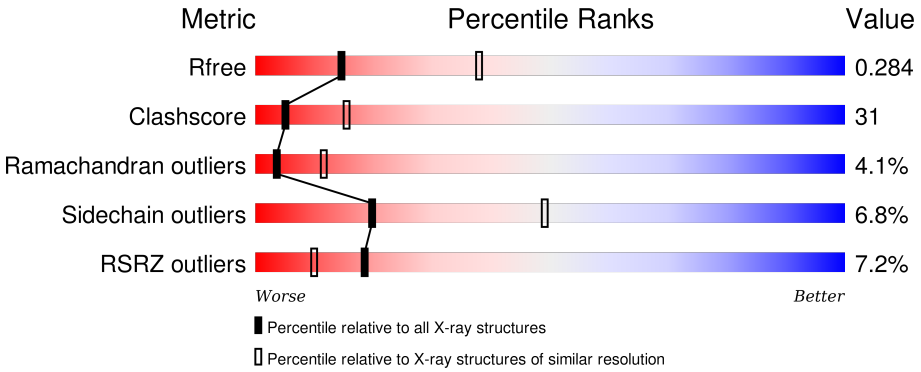
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	562	7%, 45%, 41%, 6%, 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4307 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 Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4292	2796	690	785	21	0	0	0

- Molecule 2 is water.

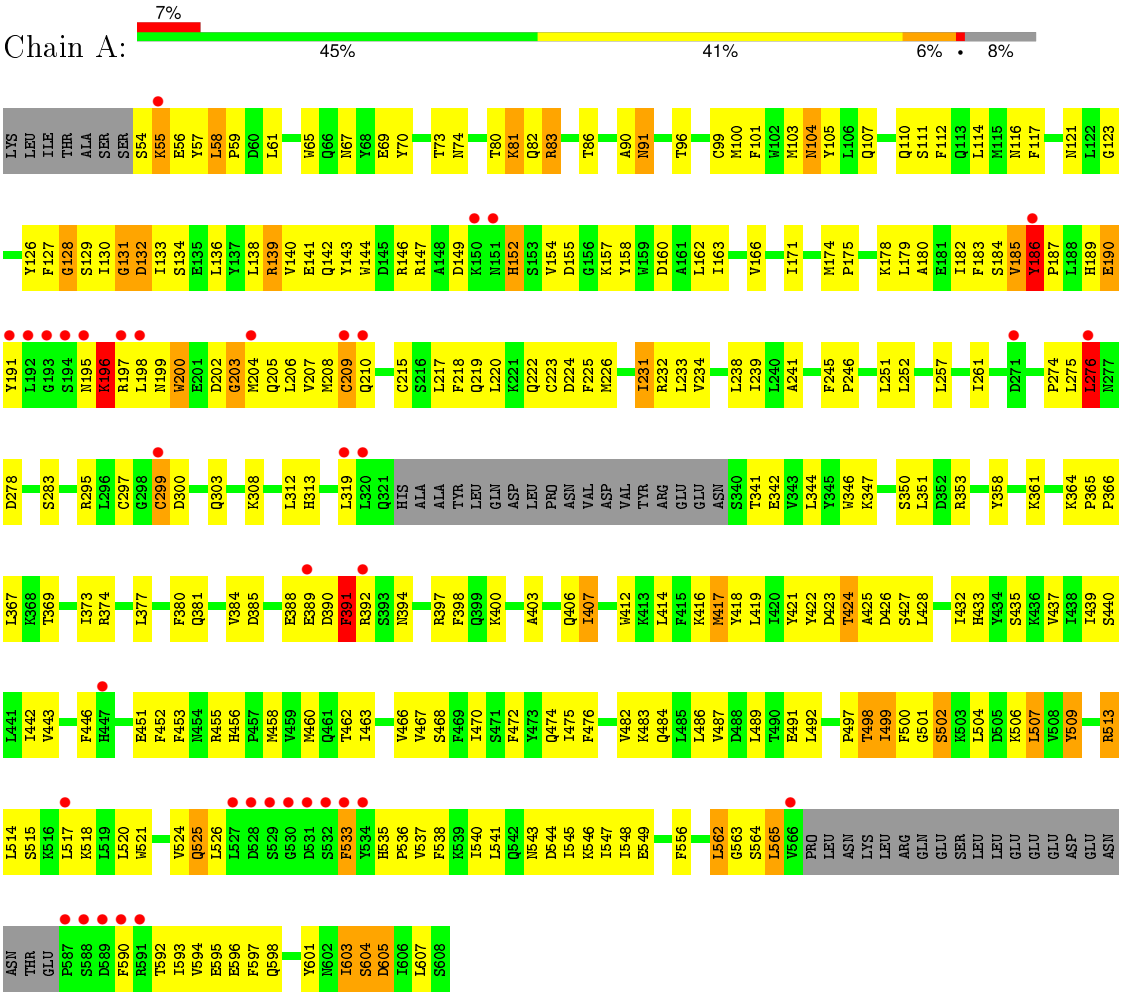
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	15	15	15	0	0

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 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: Centromere DNA-binding protein complex CBF3 subunit B

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.63Å 84.63Å 230.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.80 40.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.00-2.80) 94.2 (40.54-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.285 0.228 , 0.284	Depositor DCC
R_{free} test set	1998 reflections (9.83%)	DCC
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 20365 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4307	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

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	0.42	0/4397	0.64	1/5955 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	CYS	CA-CB-SG	-6.05	103.11	114.00

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	4292	0	4270	264	0
2	A	15	0	0	1	0
All	All	4307	0	4270	264	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 31.

All (264) 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:190:GLU:CD	1:A:191:TYR:H	1.66	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:VAL:HG21	1:A:407:ILE:HD11	1.49	0.94
1:A:499:ILE:H	1:A:499:ILE:HD13	1.31	0.93
1:A:157:LYS:HE3	1:A:222:GLN:HE22	1.36	0.90
1:A:130:ILE:HD11	1:A:162:LEU:HD11	1.52	0.89
1:A:594:VAL:HG23	1:A:595:GLU:H	1.38	0.88
1:A:157:LYS:HE3	1:A:222:GLN:NE2	1.89	0.87
1:A:203:GLY:O	1:A:207:VAL:HG23	1.78	0.84
1:A:127:PHE:CD1	1:A:131:GLY:HA2	2.14	0.82
1:A:467:VAL:HG22	1:A:489:LEU:HB3	1.62	0.80
1:A:594:VAL:HG23	1:A:595:GLU:N	1.97	0.80
1:A:195:ASN:C	1:A:197:ARG:H	1.82	0.79
1:A:126:TYR:CZ	1:A:133:ILE:HG13	2.18	0.79
1:A:55:LYS:HE3	1:A:521:TRP:HH2	1.48	0.78
1:A:443:VAL:HA	1:A:446:PHE:CE1	2.21	0.76
1:A:276:LEU:H	1:A:276:LEU:HD23	1.50	0.76
1:A:483:LYS:O	1:A:487:VAL:HG23	1.85	0.75
1:A:446:PHE:HA	1:A:451:GLU:HG2	1.68	0.74
1:A:81:LYS:HG2	1:A:83:ARG:HD3	1.69	0.74
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.53	0.74
1:A:442:ILE:CD1	1:A:463:ILE:HD11	2.17	0.74
1:A:374:ARG:HH11	1:A:374:ARG:HG2	1.53	0.73
1:A:139:ARG:CG	1:A:139:ARG:HH11	2.01	0.73
1:A:513:ARG:HG3	1:A:513:ARG:HH11	1.54	0.73
1:A:319:LEU:HD21	1:A:347:LYS:HD2	1.69	0.72
1:A:184:SER:O	1:A:187:PRO:HD2	1.90	0.72
1:A:82:GLN:C	1:A:83:ARG:HD2	2.11	0.71
1:A:58:LEU:HD12	1:A:61:LEU:HD23	1.73	0.71
1:A:543:ASN:HA	1:A:546:LYS:HG2	1.73	0.71
1:A:231:ILE:H	1:A:231:ILE:HD12	1.55	0.71
1:A:83:ARG:HD2	1:A:83:ARG:N	2.04	0.71
1:A:592:THR:O	1:A:596:GLU:HG3	1.90	0.70
1:A:536:PRO:O	1:A:540:ILE:HG13	1.93	0.69
1:A:57:TYR:CD1	1:A:58:LEU:N	2.61	0.68
1:A:158:TYR:HB3	1:A:232:ARG:NH1	2.08	0.68
1:A:385:ASP:HA	1:A:400:LYS:NZ	2.10	0.67
1:A:475:ILE:HG22	1:A:518:LYS:HB2	1.76	0.66
1:A:590:PHE:HA	1:A:593:ILE:HG12	1.77	0.66
1:A:499:ILE:CD1	1:A:499:ILE:H	2.01	0.66
1:A:366:PRO:HG2	1:A:369:THR:OG1	1.95	0.66
1:A:105:TYR:OH	1:A:183:PHE:HB3	1.95	0.66
1:A:179:LEU:HD22	1:A:205:GLN:NE2	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:O	1:A:91:ASN:HB3	1.95	0.65
1:A:439:ILE:HG23	1:A:492:LEU:HD22	1.77	0.65
1:A:446:PHE:HA	1:A:451:GLU:CG	2.27	0.64
1:A:517:LEU:HD22	1:A:537:VAL:HG13	1.80	0.64
1:A:377:LEU:HD12	1:A:414:LEU:HD22	1.80	0.64
1:A:65:TRP:HH2	1:A:468:SER:HB3	1.63	0.64
1:A:162:LEU:O	1:A:166:VAL:HG23	1.98	0.63
1:A:544:ASP:HA	1:A:603:ILE:HG12	1.79	0.63
1:A:313:HIS:HB2	1:A:346:TRP:HH2	1.62	0.63
1:A:138:LEU:O	1:A:142:GLN:HG3	1.99	0.63
1:A:499:ILE:N	1:A:499:ILE:HD13	2.09	0.62
1:A:144:TRP:HA	1:A:147:ARG:HB2	1.81	0.62
1:A:179:LEU:HD22	1:A:205:GLN:HE21	1.62	0.62
1:A:535:HIS:CG	1:A:536:PRO:HD2	2.35	0.62
1:A:391:PHE:H	1:A:391:PHE:HD1	1.45	0.62
1:A:548:ILE:CD1	1:A:607:LEU:HD21	2.30	0.62
1:A:594:VAL:CG2	1:A:595:GLU:H	2.11	0.61
1:A:419:LEU:HB2	1:A:427:SER:HB3	1.82	0.61
1:A:313:HIS:HB2	1:A:346:TRP:CH2	2.35	0.61
1:A:513:ARG:HG3	1:A:513:ARG:NH1	2.15	0.61
1:A:487:VAL:O	1:A:491:GLU:HG3	2.00	0.61
1:A:562:LEU:O	1:A:564:SER:N	2.34	0.61
1:A:546:LYS:HG3	1:A:547:ILE:HG13	1.83	0.60
1:A:533:PHE:N	1:A:533:PHE:CD1	2.69	0.60
1:A:535:HIS:HD2	1:A:537:VAL:H	1.49	0.60
1:A:202:ASP:CG	1:A:203:GLY:H	2.04	0.60
1:A:562:LEU:C	1:A:564:SER:H	2.04	0.60
1:A:543:ASN:HB3	1:A:547:ILE:HD11	1.82	0.60
1:A:200:TRP:HA	1:A:200:TRP:CE3	2.38	0.59
1:A:460:MET:HB2	1:A:500:PHE:CE1	2.37	0.59
1:A:234:VAL:O	1:A:238:LEU:HG	2.02	0.59
1:A:178:LYS:O	1:A:182:ILE:HG13	2.02	0.59
1:A:107:GLN:HB2	1:A:110:GLN:HG3	1.84	0.58
1:A:133:ILE:O	1:A:136:LEU:N	2.31	0.58
1:A:185:VAL:HB	1:A:189:HIS:NE2	2.18	0.58
1:A:129:SER:HB2	2:A:619:HOH:O	2.04	0.58
1:A:546:LYS:HG3	1:A:547:ILE:N	2.19	0.58
1:A:603:ILE:HD12	1:A:604:SER:H	1.69	0.58
1:A:502:SER:O	1:A:506:LYS:HG2	2.05	0.57
1:A:389:GLU:O	1:A:389:GLU:HG3	2.05	0.57
1:A:112:PHE:O	1:A:116:ASN:ND2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:TRP:CZ2	1:A:466:VAL:HA	2.39	0.57
1:A:160:ASP:HB3	1:A:219:GLN:OE1	2.05	0.57
1:A:594:VAL:CG2	1:A:595:GLU:N	2.68	0.57
1:A:132:ASP:OD2	1:A:134:SER:HB2	2.05	0.57
1:A:217:LEU:CD1	1:A:252:LEU:HD21	2.35	0.57
1:A:200:TRP:HE3	1:A:200:TRP:HA	1.70	0.56
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.87	0.56
1:A:391:PHE:CD1	1:A:391:PHE:N	2.73	0.56
1:A:545:ILE:O	1:A:549:GLU:HB2	2.05	0.56
1:A:54:SER:O	1:A:56:GLU:N	2.36	0.56
1:A:139:ARG:CG	1:A:139:ARG:NH1	2.64	0.56
1:A:171:ILE:HG21	1:A:208:MET:HB3	1.86	0.56
1:A:82:GLN:N	1:A:83:ARG:HH11	2.04	0.56
1:A:467:VAL:CG2	1:A:489:LEU:HB3	2.34	0.56
1:A:452:PHE:CZ	1:A:453:PHE:HE1	2.24	0.55
1:A:157:LYS:CE	1:A:222:GLN:HE22	2.15	0.55
1:A:111:SER:HA	1:A:114:LEU:HD12	1.88	0.55
1:A:195:ASN:C	1:A:197:ARG:N	2.54	0.55
1:A:215:CYS:O	1:A:219:GLN:HG3	2.06	0.55
1:A:274:PRO:CB	1:A:283:SER:HB3	2.35	0.55
1:A:202:ASP:CG	1:A:203:GLY:N	2.60	0.55
1:A:456:HIS:CE1	1:A:458:MET:HB2	2.42	0.54
1:A:70:TYR:O	1:A:74:ASN:HB3	2.07	0.54
1:A:99:CYS:O	1:A:103:MET:HG3	2.07	0.54
1:A:466:VAL:O	1:A:470:ILE:HG12	2.07	0.54
1:A:384:VAL:CG2	1:A:407:ILE:HD11	2.32	0.54
1:A:209:CYS:SG	1:A:209:CYS:O	2.64	0.54
1:A:313:HIS:HD2	1:A:353:ARG:HH11	1.54	0.54
1:A:261:ILE:HD12	1:A:312:LEU:HB2	1.89	0.54
1:A:548:ILE:HD13	1:A:607:LEU:HD21	1.90	0.54
1:A:384:VAL:HG21	1:A:407:ILE:CD1	2.32	0.54
1:A:57:TYR:HH	1:A:521:TRP:HZ2	1.56	0.53
1:A:515:SER:O	1:A:518:LYS:HB3	2.08	0.53
1:A:472:PHE:O	1:A:475:ILE:HG12	2.09	0.53
1:A:69:GLU:O	1:A:73:THR:OG1	2.18	0.53
1:A:231:ILE:CD1	1:A:231:ILE:H	2.17	0.53
1:A:474:GLN:HG2	1:A:482:VAL:HG12	1.90	0.53
1:A:126:TYR:CE1	1:A:133:ILE:HG13	2.42	0.53
1:A:374:ARG:NH1	1:A:374:ARG:HG2	2.21	0.53
1:A:474:GLN:HG3	1:A:486:LEU:HD22	1.91	0.53
1:A:536:PRO:HD3	1:A:590:PHE:CD1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:CD	1:A:191:TYR:N	2.49	0.53
1:A:509:TYR:CD1	1:A:509:TYR:C	2.82	0.53
1:A:274:PRO:HB3	1:A:283:SER:HB3	1.91	0.52
1:A:498:THR:C	1:A:500:PHE:N	2.62	0.52
1:A:524:VAL:HG12	1:A:525:GLN:N	2.25	0.52
1:A:80:THR:O	1:A:81:LYS:HB2	2.10	0.52
1:A:543:ASN:C	1:A:547:ILE:HD12	2.30	0.52
1:A:498:THR:C	1:A:500:PHE:H	2.11	0.52
1:A:96:THR:O	1:A:100:MET:HB2	2.10	0.52
1:A:157:LYS:CE	1:A:222:GLN:NE2	2.69	0.52
1:A:455:ARG:HG2	1:A:499:ILE:CG1	2.40	0.51
1:A:198:LEU:HD23	1:A:202:ASP:OD2	2.09	0.51
1:A:351:LEU:HD22	1:A:373:ILE:HG23	1.92	0.51
1:A:341:THR:HG23	1:A:342:GLU:N	2.25	0.51
1:A:204:MET:HA	1:A:207:VAL:HG23	1.92	0.51
1:A:140:VAL:O	1:A:143:TYR:HB3	2.10	0.51
1:A:593:ILE:HA	1:A:596:GLU:OE2	2.10	0.51
1:A:117:PHE:CZ	1:A:175:PRO:HD3	2.46	0.51
1:A:381:GLN:O	1:A:385:ASP:OD1	2.29	0.50
1:A:437:VAL:O	1:A:440:SER:HB3	2.11	0.50
1:A:358:TYR:HA	1:A:361:LYS:HB2	1.93	0.50
1:A:535:HIS:CD2	1:A:537:VAL:H	2.27	0.50
1:A:61:LEU:HD21	1:A:476:PHE:CE2	2.47	0.50
1:A:160:ASP:O	1:A:163:ILE:HG12	2.11	0.50
1:A:543:ASN:HD22	1:A:598:GLN:NE2	2.08	0.50
1:A:206:LEU:HG	1:A:206:LEU:O	2.12	0.50
1:A:123:GLY:HA2	1:A:126:TYR:CE2	2.47	0.50
1:A:195:ASN:HB2	1:A:197:ARG:HB3	1.94	0.50
1:A:114:LEU:HD23	1:A:174:MET:CE	2.41	0.50
1:A:231:ILE:N	1:A:231:ILE:HD12	2.23	0.50
1:A:275:LEU:O	1:A:278:ASP:HB2	2.12	0.50
1:A:603:ILE:HD12	1:A:604:SER:N	2.27	0.49
1:A:497:PRO:HB2	1:A:499:ILE:HD11	1.94	0.49
1:A:540:ILE:HD13	1:A:597:PHE:CD2	2.46	0.49
1:A:455:ARG:HG2	1:A:499:ILE:HD11	1.94	0.49
1:A:424:THR:HG22	1:A:425:ALA:H	1.77	0.49
1:A:131:GLY:O	1:A:132:ASP:C	2.50	0.49
1:A:55:LYS:HE3	1:A:521:TRP:CH2	2.37	0.49
1:A:133:ILE:O	1:A:134:SER:C	2.50	0.49
1:A:442:ILE:HD12	1:A:463:ILE:HD11	1.92	0.49
1:A:319:LEU:HD13	1:A:350:SER:OG	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:O	1:A:432:ILE:HG13	2.12	0.49
1:A:403:ALA:O	1:A:407:ILE:HG13	2.12	0.49
1:A:513:ARG:NH1	1:A:601:TYR:O	2.40	0.49
1:A:564:SER:C	1:A:565:LEU:O	2.46	0.49
1:A:208:MET:C	1:A:210:GLN:N	2.66	0.49
1:A:185:VAL:HG21	1:A:199:ASN:OD1	2.12	0.49
1:A:220:LEU:HD13	1:A:233:LEU:CD1	2.43	0.49
1:A:146:ARG:HD2	1:A:152:HIS:NE2	2.28	0.48
1:A:297:CYS:HB3	1:A:346:TRP:CZ3	2.49	0.48
1:A:186:TYR:HB3	1:A:187:PRO:HD3	1.95	0.48
1:A:425:ALA:O	1:A:426:ASP:HB2	2.14	0.48
1:A:513:ARG:HD3	1:A:514:LEU:HD12	1.95	0.47
1:A:433:HIS:O	1:A:437:VAL:HG23	2.14	0.47
1:A:452:PHE:HA	1:A:455:ARG:HD3	1.95	0.47
1:A:406:GLN:HG2	1:A:458:MET:SD	2.54	0.47
1:A:544:ASP:HB3	1:A:603:ILE:HG21	1.95	0.47
1:A:127:PHE:CE1	1:A:131:GLY:HA2	2.49	0.47
1:A:526:LEU:HD11	1:A:533:PHE:HB3	1.95	0.47
1:A:597:PHE:CE1	1:A:601:TYR:HD2	2.33	0.47
1:A:347:LYS:O	1:A:350:SER:HB3	2.14	0.46
1:A:198:LEU:N	1:A:198:LEU:HD12	2.31	0.46
1:A:67:ASN:N	1:A:67:ASN:HD22	2.13	0.46
1:A:61:LEU:HD21	1:A:476:PHE:CD2	2.51	0.46
1:A:377:LEU:CD1	1:A:414:LEU:HD22	2.46	0.46
1:A:535:HIS:CD2	1:A:536:PRO:HD2	2.51	0.46
1:A:603:ILE:O	1:A:605:ASP:N	2.49	0.46
1:A:186:TYR:CD1	1:A:196:LYS:NZ	2.83	0.46
1:A:117:PHE:O	1:A:121:ASN:HB2	2.16	0.46
1:A:455:ARG:HG3	1:A:497:PRO:HG3	1.98	0.46
1:A:196:LYS:HD2	1:A:196:LYS:O	2.15	0.46
1:A:299:CYS:O	1:A:303:GLN:HG3	2.16	0.46
1:A:412:TRP:HE1	1:A:435:SER:HG	1.64	0.45
1:A:104:ASN:HD22	1:A:104:ASN:C	2.19	0.45
1:A:186:TYR:CB	1:A:187:PRO:CD	2.94	0.45
1:A:208:MET:C	1:A:210:GLN:H	2.18	0.45
1:A:197:ARG:HG2	1:A:197:ARG:O	2.17	0.45
1:A:274:PRO:HB2	1:A:283:SER:HB3	1.98	0.45
1:A:154:VAL:HG13	1:A:223:CYS:HB3	1.99	0.45
1:A:394:ASN:OD1	1:A:397:ARG:NH2	2.50	0.44
1:A:101:PHE:O	1:A:104:ASN:HB3	2.17	0.44
1:A:61:LEU:HD21	1:A:476:PHE:CZ	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:O	1:A:241:ALA:HB3	2.17	0.44
1:A:364:LYS:HE2	1:A:422:TYR:CZ	2.52	0.44
1:A:507:LEU:HD22	1:A:507:LEU:O	2.17	0.44
1:A:590:PHE:HA	1:A:593:ILE:CG1	2.46	0.44
1:A:138:LEU:O	1:A:141:GLU:HB3	2.18	0.44
1:A:526:LEU:HD13	1:A:535:HIS:HB2	1.99	0.44
1:A:186:TYR:HB3	1:A:187:PRO:CD	2.48	0.43
1:A:158:TYR:CB	1:A:232:ARG:NH1	2.77	0.43
1:A:195:ASN:O	1:A:197:ARG:N	2.51	0.43
1:A:155:ASP:OD1	1:A:232:ARG:NH2	2.51	0.43
1:A:127:PHE:O	1:A:128:GLY:C	2.57	0.43
1:A:412:TRP:CZ3	1:A:416:LYS:HD3	2.53	0.43
1:A:435:SER:O	1:A:439:ILE:HG13	2.18	0.43
1:A:452:PHE:CZ	1:A:453:PHE:CE1	3.06	0.43
1:A:257:LEU:HD21	1:A:300:ASP:HA	2.00	0.43
1:A:407:ILE:HG13	1:A:407:ILE:H	1.45	0.43
1:A:543:ASN:O	1:A:547:ILE:HD12	2.19	0.43
1:A:220:LEU:HD13	1:A:233:LEU:HD12	2.01	0.43
1:A:82:GLN:N	1:A:83:ARG:NH1	2.66	0.43
1:A:127:PHE:O	1:A:129:SER:N	2.52	0.43
1:A:462:THR:O	1:A:466:VAL:HG23	2.19	0.43
1:A:217:LEU:HD13	1:A:252:LEU:HD21	2.00	0.43
1:A:367:LEU:HD11	1:A:418:TYR:HE1	1.84	0.42
1:A:423:ASP:O	1:A:423:ASP:CG	2.56	0.42
1:A:365:PRO:O	1:A:366:PRO:C	2.55	0.42
1:A:190:GLU:O	1:A:191:TYR:C	2.58	0.42
1:A:562:LEU:C	1:A:564:SER:N	2.71	0.42
1:A:245:PHE:N	1:A:246:PRO:HD2	2.34	0.42
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.71	0.42
1:A:341:THR:CG2	1:A:342:GLU:N	2.83	0.42
1:A:224:ASP:O	1:A:226:MET:N	2.53	0.42
1:A:198:LEU:HD22	1:A:204:MET:HE3	2.02	0.41
1:A:144:TRP:O	1:A:147:ARG:HB3	2.20	0.41
1:A:344:LEU:CD1	1:A:380:PHE:HD1	2.33	0.41
1:A:535:HIS:HB3	1:A:538:PHE:CD1	2.55	0.41
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.83	0.41
1:A:364:LYS:HE2	1:A:422:TYR:OH	2.21	0.41
1:A:384:VAL:HG11	1:A:407:ILE:HD11	2.02	0.41
1:A:96:THR:HG22	1:A:218:PHE:HE1	1.86	0.41
1:A:180:ALA:HA	1:A:200:TRP:CD1	2.56	0.41
1:A:424:THR:HG22	1:A:425:ALA:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MET:HA	1:A:207:VAL:CG2	2.51	0.41
1:A:82:GLN:C	1:A:83:ARG:HH11	2.24	0.41
1:A:543:ASN:ND2	1:A:598:GLN:NE2	2.68	0.41
1:A:603:ILE:C	1:A:605:ASP:N	2.73	0.41
1:A:390:ASP:C	1:A:392:ARG:H	2.24	0.41
1:A:452:PHE:HA	1:A:455:ARG:CD	2.51	0.41
1:A:139:ARG:HD3	1:A:142:GLN:OE1	2.21	0.41
1:A:295:ARG:HD2	1:A:295:ARG:HA	1.97	0.41
1:A:58:LEU:O	1:A:61:LEU:HB3	2.21	0.40
1:A:535:HIS:O	1:A:538:PHE:HB2	2.21	0.40
1:A:257:LEU:O	1:A:261:ILE:HG12	2.21	0.40
1:A:417:MET:HG3	1:A:421:TYR:CE2	2.57	0.40
1:A:239:ILE:HA	1:A:239:ILE:HD13	1.91	0.40
1:A:374:ARG:CG	1:A:374:ARG:NH1	2.84	0.40
1:A:184:SER:O	1:A:186:TYR:N	2.55	0.40
1:A:346:TRP:O	1:A:347:LYS:C	2.59	0.40
1:A:185:VAL:HB	1:A:189:HIS:CD2	2.57	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	511/562 (91%)	441 (86%)	49 (10%)	21 (4%)	3 11

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	388	GLU
1	A	55	LYS
1	A	131	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	225	PHE
1	A	501	GLY
1	A	563	GLY
1	A	81	LYS
1	A	91	ASN
1	A	128	GLY
1	A	276	LEU
1	A	565	LEU
1	A	196	LYS
1	A	391	PHE
1	A	424	THR
1	A	502	SER
1	A	604	SER
1	A	58	LEU
1	A	186	TYR
1	A	185	VAL
1	A	203	GLY

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	483/525 (92%)	450 (93%)	33 (7%)	20 49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	86	THR
1	A	104	ASN
1	A	139	ARG
1	A	149	ASP
1	A	152	HIS
1	A	186	TYR
1	A	190	GLU
1	A	196	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	200	TRP
1	A	209	CYS
1	A	231	ILE
1	A	276	LEU
1	A	308	LYS
1	A	391	PHE
1	A	398	PHE
1	A	407	ILE
1	A	417	MET
1	A	484	GLN
1	A	498	THR
1	A	499	ILE
1	A	504	LEU
1	A	507	LEU
1	A	509	TYR
1	A	513	ARG
1	A	520	LEU
1	A	525	GLN
1	A	533	PHE
1	A	541	LEU
1	A	556	PHE
1	A	562	LEU
1	A	603	ILE
1	A	605	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	104	ASN
1	A	121	ASN
1	A	205	GLN
1	A	222	GLN
1	A	399	GLN
1	A	454	ASN
1	A	535	HIS
1	A	598	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	517/562 (91%)	0.43	37 (7%) 18 10	53, 91, 163, 201	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	ASP	6.9
1	A	209	CYS	6.0
1	A	590	PHE	5.8
1	A	447	HIS	5.3
1	A	198	LEU	5.3
1	A	530	GLY	5.0
1	A	528	ASP	5.0
1	A	192	LEU	4.8
1	A	197	ARG	4.8
1	A	529	SER	4.7
1	A	587	PRO	4.7
1	A	191	TYR	4.5
1	A	194	SER	4.2
1	A	150	LYS	4.1
1	A	588	SER	3.9
1	A	532	SER	3.8
1	A	566	VAL	3.8
1	A	527	LEU	3.7
1	A	392	ARG	3.7
1	A	195	ASN	3.5
1	A	320	LEU	3.4
1	A	591	ARG	3.1
1	A	389	GLU	3.1
1	A	186	TYR	3.0
1	A	299	CYS	3.0
1	A	151	ASN	2.9
1	A	204	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	2.8
1	A	319	LEU	2.8
1	A	533	PHE	2.7
1	A	276	LEU	2.5
1	A	589	ASP	2.5
1	A	271	ASP	2.4
1	A	210	GLN	2.3
1	A	517	LEU	2.2
1	A	534	TYR	2.1
1	A	193	GLY	2.1

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

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

6.3 Carbohydrates

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.