Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:53 am BST

PDB ID	:	1ZZD
Title	:	Structures of Yeast Ribonucleotide Reductase I
Authors	:	Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.
Deposited on	:	2005-06-13
Resolution	:	2.60 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
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:

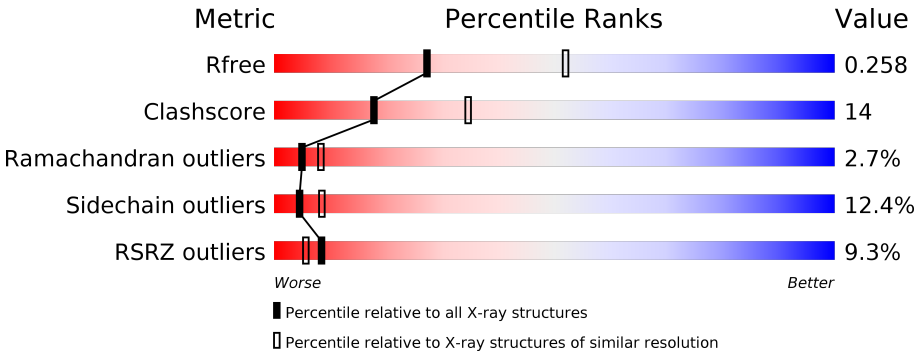
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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 <=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	888	6%, 47%, 21%, ·, 28%
2	B	9	44%, 56%, 11%, 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5241 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 Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	640	5128	3272	865	960	31	0	0	0

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase small chain 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	55	34	7	14	0	0	0

- Molecule 3 is water.

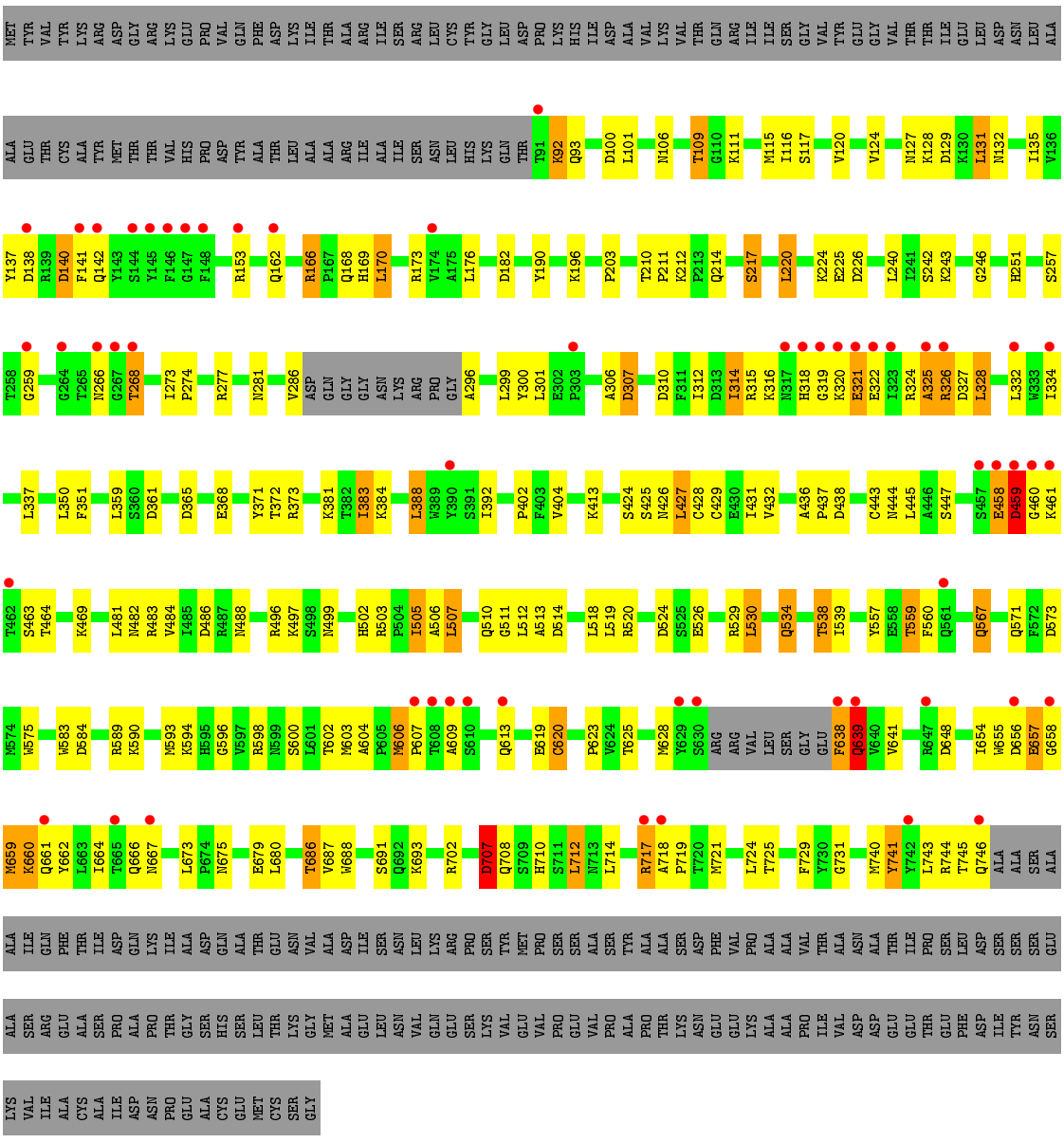
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0

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.

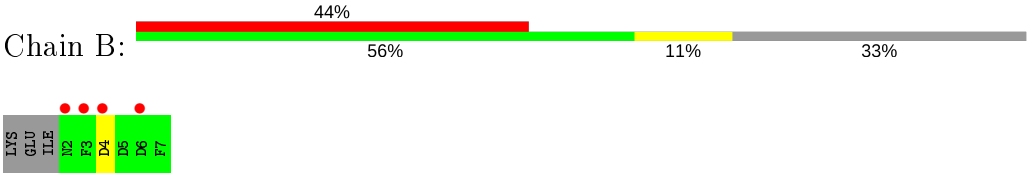
- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

Chain A:



• Molecule 2: Ribonucleoside-diphosphate reductase small chain 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	108.32Å 117.68Å 64.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 24.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.60) 99.7 (24.60-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.201 , 0.260 0.199 , 0.258	Depositor DCC
R_{free} test set	2626 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5241	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.333 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	0.77	0/5247	0.92	13/7103 (0.2%)
2	B	0.80	0/56	1.54	1/73 (1.4%)
All	All	0.77	0/5303	0.93	14/7176 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	ASP	CB-CG-OD2	7.34	124.90	118.30
2	B	4	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	100	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	182	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	140	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	365	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	507	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	A	712	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	310	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	584	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	307	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	129	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	573	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	459	ASP	CB-CG-OD2	5.01	122.81	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	5128	0	5057	140	0
2	B	55	0	35	0	0
3	A	58	0	0	2	0
All	All	5241	0	5092	140	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 (140) 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:383:ILE:CD1	1:A:383:ILE:CG1	1.76	1.57
1:A:326:ARG:HH11	1:A:326:ARG:HG3	1.18	1.06
1:A:538:THR:HB	1:A:583:TRP:NE1	1.77	0.99
1:A:538:THR:HB	1:A:583:TRP:HE1	1.25	0.99
1:A:638:PHE:O	1:A:639:GLN:HB3	1.66	0.95
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.34	0.92
1:A:567:GLN:CA	1:A:567:GLN:HE21	1.89	0.85
1:A:589:ARG:O	1:A:593:MET:HG3	1.76	0.85
1:A:557:TYR:CD1	1:A:559:THR:HG22	2.14	0.81
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.66	0.78
1:A:654:ILE:HG21	1:A:675:ASN:HD22	1.49	0.77
1:A:326:ARG:CG	1:A:326:ARG:HH11	1.97	0.77
1:A:639:GLN:NE2	1:A:660:LYS:HE3	2.00	0.77
1:A:520:ARG:NH2	1:A:648:ASP:OD2	2.18	0.76
1:A:717:ARG:O	1:A:719:PRO:HD3	1.87	0.74
1:A:217:SER:HB3	1:A:445:LEU:HD12	1.69	0.74
1:A:217:SER:CB	1:A:445:LEU:HD12	2.18	0.74
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.20	0.73
1:A:666:GLN:O	1:A:667:ASN:HB2	1.90	0.70
1:A:427:LEU:O	1:A:427:LEU:HD12	1.92	0.70
1:A:296:ALA:HB3	1:A:427:LEU:HD21	1.73	0.69
1:A:259:GLY:HA2	1:A:268:THR:OG1	1.92	0.69
1:A:602:THR:N	1:A:707:ASP:OD2	2.25	0.69
1:A:326:ARG:NH1	1:A:326:ARG:HG3	1.93	0.69
1:A:557:TYR:CE1	1:A:559:THR:HG22	2.28	0.69
1:A:557:TYR:HD1	1:A:559:THR:HG22	1.59	0.68
1:A:530:LEU:O	1:A:534:GLN:HG2	1.94	0.67
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.75	0.67
1:A:426:ASN:ND2	1:A:428:CYS:H	1.93	0.67
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.76	0.67
1:A:166:ARG:HB2	1:A:169:HIS:CE1	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:GLU:C	1:A:659:MET:H	2.00	0.65
1:A:688:TRP:HB3	1:A:717:ARG:HH11	1.62	0.64
1:A:388:LEU:O	1:A:392:ILE:HG12	1.97	0.64
1:A:445:LEU:HD23	1:A:506:ALA:HB3	1.78	0.64
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.14	0.62
1:A:447:SER:HB3	1:A:606:MET:CE	2.30	0.62
1:A:445:LEU:HD23	1:A:506:ALA:CB	2.29	0.62
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.35	0.61
1:A:745:THR:O	1:A:746:GLN:HB2	2.01	0.61
1:A:567:GLN:NE2	1:A:567:GLN:HA	2.11	0.60
1:A:538:THR:CB	1:A:583:TRP:HE1	2.10	0.59
1:A:383:ILE:HD12	1:A:384:LYS:H	1.67	0.59
1:A:510:GLN:HA	1:A:620:CYS:HA	1.83	0.59
1:A:660:LYS:O	1:A:664:ILE:HG12	2.01	0.59
1:A:242:SER:HB3	1:A:286:VAL:HG21	1.85	0.58
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.18	0.58
1:A:719:PRO:HG3	1:A:745:THR:OG1	2.04	0.58
1:A:534:GLN:O	1:A:538:THR:HG22	2.03	0.57
1:A:654:ILE:HG21	1:A:675:ASN:ND2	2.16	0.57
1:A:320:LYS:NZ	1:A:320:LYS:HB2	2.20	0.57
1:A:324:ARG:O	1:A:325:ALA:HB2	2.04	0.57
1:A:444:ASN:HD21	1:A:499:ASN:HD21	1.53	0.56
1:A:534:GLN:O	1:A:538:THR:CG2	2.54	0.56
1:A:109:THR:HG23	1:A:111:LYS:HG3	1.86	0.55
1:A:299:LEU:HD11	1:A:328:LEU:HD12	1.87	0.55
1:A:120:VAL:O	1:A:124:VAL:HG23	2.07	0.55
1:A:116:ILE:HG22	1:A:117:SER:O	2.07	0.55
1:A:740:MET:HG2	1:A:741:TYR:O	2.05	0.55
1:A:486:ASP:OD1	1:A:503:ARG:NH2	2.39	0.55
1:A:140:ASP:OD1	1:A:166:ARG:NH1	2.40	0.55
1:A:686:THR:CG2	1:A:688:TRP:HD1	2.21	0.54
1:A:106:ASN:OD1	1:A:109:THR:CG2	2.56	0.54
1:A:368:GLU:O	1:A:372:THR:HB	2.08	0.54
1:A:211:PRO:O	1:A:212:LYS:HD3	2.08	0.53
1:A:539:ILE:HG22	1:A:603:MET:SD	2.49	0.53
1:A:484:VAL:O	1:A:488:ASN:HB2	2.09	0.53
1:A:220:LEU:HD13	1:A:425:SER:O	2.09	0.53
1:A:101:LEU:HD22	1:A:115:MET:CE	2.39	0.52
1:A:300:TYR:OH	1:A:425:SER:HB3	2.10	0.51
1:A:203:PRO:HG2	1:A:217:SER:HA	1.93	0.51
1:A:686:THR:HG22	1:A:688:TRP:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:SER:HB3	1:A:606:MET:HE3	1.93	0.51
1:A:210:THR:HB	1:A:211:PRO:HD2	1.93	0.51
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.92	0.51
1:A:662:TYR:CE1	1:A:666:GLN:HG3	2.46	0.50
1:A:688:TRP:HB3	1:A:717:ARG:NH1	2.26	0.50
1:A:428:CYS:O	1:A:429:CYS:HB2	2.11	0.49
1:A:731:GLY:HA3	3:A:939:HOH:O	2.12	0.49
1:A:257:SER:HA	1:A:307:ASP:OD2	2.13	0.48
1:A:438:ASP:OD1	1:A:497:LYS:NZ	2.44	0.48
1:A:217:SER:HB3	1:A:445:LEU:CD1	2.39	0.48
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.31	0.48
1:A:567:GLN:N	1:A:567:GLN:HE21	2.11	0.48
1:A:447:SER:HB3	1:A:606:MET:HE1	1.96	0.48
1:A:625:THR:HA	1:A:687:VAL:HG12	1.94	0.48
1:A:109:THR:HG23	1:A:111:LYS:H	1.79	0.48
1:A:662:TYR:CZ	1:A:666:GLN:HG3	2.48	0.48
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.96	0.48
1:A:604:ALA:HB2	1:A:708:GLN:HB2	1.95	0.47
1:A:557:TYR:CE1	1:A:559:THR:CG2	2.96	0.47
1:A:436:ALA:HB1	1:A:437:PRO:HD2	1.95	0.47
1:A:351:PHE:HE1	1:A:371:TYR:CE1	2.33	0.47
1:A:101:LEU:HD22	1:A:115:MET:HE2	1.97	0.46
1:A:628:MET:HB3	1:A:628:MET:HE2	1.78	0.46
1:A:657:GLU:C	1:A:659:MET:N	2.69	0.46
1:A:170:LEU:C	1:A:170:LEU:CD1	2.83	0.46
1:A:224:LYS:O	1:A:225:GLU:HB2	2.15	0.46
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.31	0.46
1:A:92:LYS:HG3	1:A:92:LYS:O	2.15	0.46
1:A:606:MET:HB2	1:A:607:PRO:CD	2.47	0.45
1:A:654:ILE:C	1:A:656:ASP:H	2.19	0.45
1:A:324:ARG:O	1:A:325:ALA:CB	2.64	0.45
1:A:557:TYR:CE2	1:A:600:SER:HA	2.51	0.45
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.15	0.45
1:A:459:ASP:HB3	1:A:460:GLY:H	1.42	0.45
1:A:725:THR:O	1:A:729:PHE:HD1	2.00	0.45
1:A:659:MET:HE1	1:A:673:LEU:HD13	1.99	0.44
1:A:567:GLN:CA	1:A:567:GLN:NE2	2.63	0.44
1:A:717:ARG:O	1:A:719:PRO:CD	2.62	0.44
1:A:659:MET:HE1	1:A:673:LEU:CD1	2.48	0.44
1:A:638:PHE:HB3	1:A:639:GLN:H	1.55	0.44
1:A:513:ALA:HB2	1:A:623:PRO:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG22	1:A:402:PRO:HG3	1.99	0.43
1:A:557:TYR:HE1	1:A:559:THR:CG2	2.31	0.43
1:A:463:SER:HB3	1:A:519:LEU:HD23	2.01	0.43
1:A:273:ILE:HD12	1:A:314:ILE:HD11	2.01	0.43
1:A:315:ARG:HH12	1:A:327:ASP:HA	1.83	0.43
1:A:648:ASP:HB3	1:A:680:LEU:HD11	2.01	0.43
1:A:273:ILE:HB	1:A:274:PRO:HD3	2.01	0.43
1:A:316:LYS:HD3	1:A:318:HIS:HE2	1.84	0.42
1:A:505:ILE:HD13	1:A:505:ILE:HA	1.67	0.42
1:A:413:LYS:HE3	1:A:575:TRP:CE2	2.54	0.42
1:A:251:HIS:HB3	1:A:424:SER:HB3	2.00	0.42
1:A:483:ARG:HD2	3:A:906:HOH:O	2.19	0.42
1:A:431:ILE:HG13	1:A:443:CYS:SG	2.59	0.41
1:A:511:GLY:HA2	1:A:514:ASP:OD2	2.20	0.41
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.43	0.41
1:A:657:GLU:OE2	1:A:660:LYS:HB3	2.21	0.41
1:A:520:ARG:HH12	1:A:680:LEU:CD2	2.33	0.41
1:A:526:GLU:OE2	1:A:529:ARG:NH1	2.54	0.41
1:A:314:ILE:HD13	1:A:314:ILE:HA	1.73	0.41
1:A:557:TYR:HB3	1:A:598:ARG:O	2.21	0.41
1:A:135:ILE:HG21	1:A:137:TYR:CZ	2.56	0.41
1:A:557:TYR:CZ	1:A:600:SER:HA	2.56	0.41
1:A:240:LEU:O	1:A:243:LYS:HB3	2.20	0.40
1:A:686:THR:CG2	1:A:688:TRP:CD1	3.03	0.40
1:A:691:SER:C	1:A:693:LYS:H	2.25	0.40
1:A:128:LYS:O	1:A:132:ASN:ND2	2.55	0.40
1:A:220:LEU:N	1:A:220:LEU:HD23	2.36	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	634/888 (71%)	568 (90%)	49 (8%)	17 (3%)	5 8
2	B	4/9 (44%)	3 (75%)	1 (25%)	0	100 100
All	All	638/897 (71%)	571 (90%)	50 (8%)	17 (3%)	5 8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLU
1	A	325	ALA
1	A	458	GLU
1	A	459	ASP
1	A	639	GLN
1	A	319	GLY
1	A	619	GLU
1	A	92	LYS
1	A	246	GLY
1	A	620	CYS
1	A	707	ASP
1	A	741	TYR
1	A	655	TRP
1	A	93	GLN
1	A	609	ALA
1	A	718	ALA
1	A	658	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	557/761 (73%)	487 (87%)	70 (13%)	4 8
2	B	6/9 (67%)	6 (100%)	0	100 100
All	All	563/770 (73%)	493 (88%)	70 (12%)	4 8

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	131	LEU
1	A	138	ASP
1	A	141	PHE
1	A	142	GLN
1	A	153	ARG
1	A	162	GLN
1	A	166	ARG
1	A	170	LEU
1	A	176	LEU
1	A	196	LYS
1	A	214	GLN
1	A	217	SER
1	A	220	LEU
1	A	266	ASN
1	A	268	THR
1	A	277	ARG
1	A	281	ASN
1	A	301	LEU
1	A	314	ILE
1	A	321	GLU
1	A	322	GLU
1	A	326	ARG
1	A	328	LEU
1	A	337	LEU
1	A	359	LEU
1	A	361	ASP
1	A	373	ARG
1	A	381	LYS
1	A	383	ILE
1	A	388	LEU
1	A	427	LEU
1	A	432	VAL
1	A	458	GLU
1	A	461	LYS
1	A	464	THR
1	A	469	LYS
1	A	496	ARG
1	A	505	ILE
1	A	507	LEU
1	A	512	LEU
1	A	518	LEU
1	A	524	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	530	LEU
1	A	534	GLN
1	A	538	THR
1	A	559	THR
1	A	567	GLN
1	A	571	GLN
1	A	590	LYS
1	A	594	LYS
1	A	606	MET
1	A	613	GLN
1	A	638	PHE
1	A	639	GLN
1	A	641	VAL
1	A	657	GLU
1	A	659	MET
1	A	660	LYS
1	A	661	GLN
1	A	679	GLU
1	A	686	THR
1	A	707	ASP
1	A	712	LEU
1	A	714	LEU
1	A	717	ARG
1	A	721	MET
1	A	724	LEU
1	A	743	LEU
1	A	744	ARG

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	162	GLN
1	A	168	GLN
1	A	251	HIS
1	A	270	ASN
1	A	317	ASN
1	A	444	ASN
1	A	534	GLN
1	A	567	GLN
1	A	618	ASN
1	A	639	GLN
1	A	661	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	675	ASN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN

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	640/888 (72%)	0.18	56 (8%)	10	7	26, 41, 81, 96	0
2	B	6/9 (66%)	2.27	4 (66%)	0	0	58, 74, 82, 83	0
All	All	646/897 (72%)	0.20	60 (9%)	8	6	26, 41, 81, 96	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	PHE	7.4
1	A	318	HIS	7.3
1	A	638	PHE	6.8
1	A	458	GLU	6.1
1	A	317	ASN	5.8
1	A	321	GLU	5.7
1	A	91	THR	5.7
1	A	459	ASP	5.6
1	A	609	ALA	5.4
1	A	145	TYR	5.2
1	A	630	SER	5.1
1	A	322	GLU	5.0
1	A	457	SER	5.0
1	A	460	GLY	4.6
1	A	266	ASN	4.6
1	A	656	ASP	3.9
1	A	461	LYS	3.9
1	A	462	THR	3.8
1	A	323	ILE	3.8
1	A	326	ARG	3.7
1	A	144	SER	3.7
1	A	267	GLY	3.4
1	A	319	GLY	3.4
1	A	661	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	639	GLN	3.3
1	A	717	ARG	3.2
2	B	6	ASP	3.2
1	A	148	PHE	3.1
1	A	264	GLY	3.1
2	B	3	PHE	3.1
1	A	610	SER	3.1
1	A	162	GLN	3.0
1	A	607	PRO	2.9
1	A	320	LYS	2.9
1	A	647	ARG	2.8
1	A	629	TYR	2.8
1	A	742	TYR	2.8
1	A	141	PHE	2.8
1	A	268	THR	2.7
1	A	665	THR	2.7
2	B	4	ASP	2.7
1	A	390	TYR	2.6
1	A	608	THR	2.4
1	A	658	GLY	2.3
2	B	2	ASN	2.3
1	A	142	GLN	2.3
1	A	746	GLN	2.2
1	A	325	ALA	2.2
1	A	718	ALA	2.2
1	A	332	LEU	2.2
1	A	153	ARG	2.2
1	A	667	ASN	2.2
1	A	174	VAL	2.2
1	A	561	GLN	2.2
1	A	334	ILE	2.1
1	A	259	GLY	2.1
1	A	147	GLY	2.1
1	A	613	GLN	2.1
1	A	303	PRO	2.0
1	A	138	ASP	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

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.