WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:46 PM GMT

PDB ID	:	3UXN
Title	:	Crystal Structure of Rat DNA Polymerase Beta, Wild Type Apoenzyme
Authors	:	Gridley, C.L.; Firbank, S.; Jaeger, J.
Deposited on	:	2011-12-05
Resolution	:	2.50 Å(reported)

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

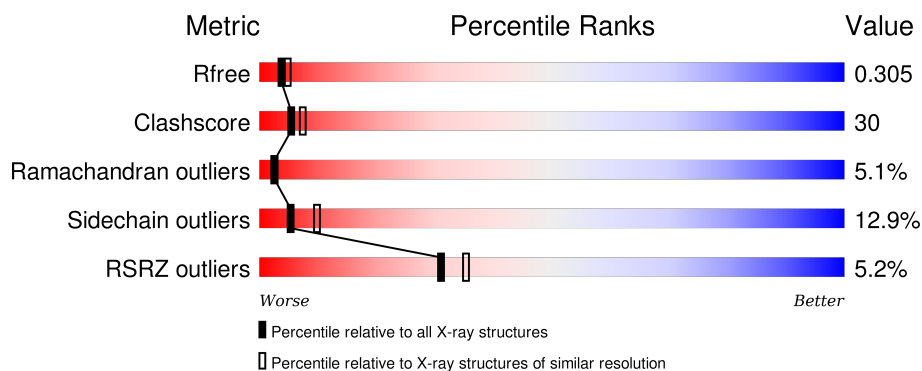|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 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	Percentile Ranks	Value
Rfree		0.305
Clashscore		30
Ramachandran outliers		5.1%
Sidechain outliers		12.9%
RSRZ outliers		5.2%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	335	4% / 55% 36% 6% · ·
1	B	335	7% / 44% 40% 11% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5379 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 DNA polymerase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2610	1647	461	493	9			
1	B	325	Total	C	N	O	S	0	0	0
			2610	1647	461	493	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	64	Total	O	0	0
			64	64		

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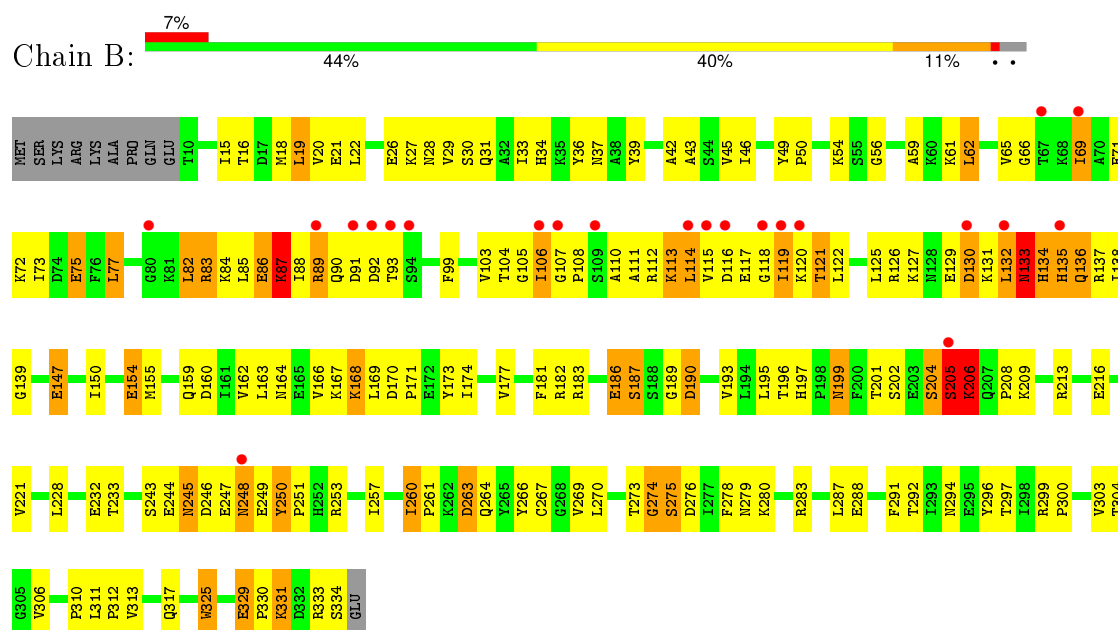 least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA polymerase beta
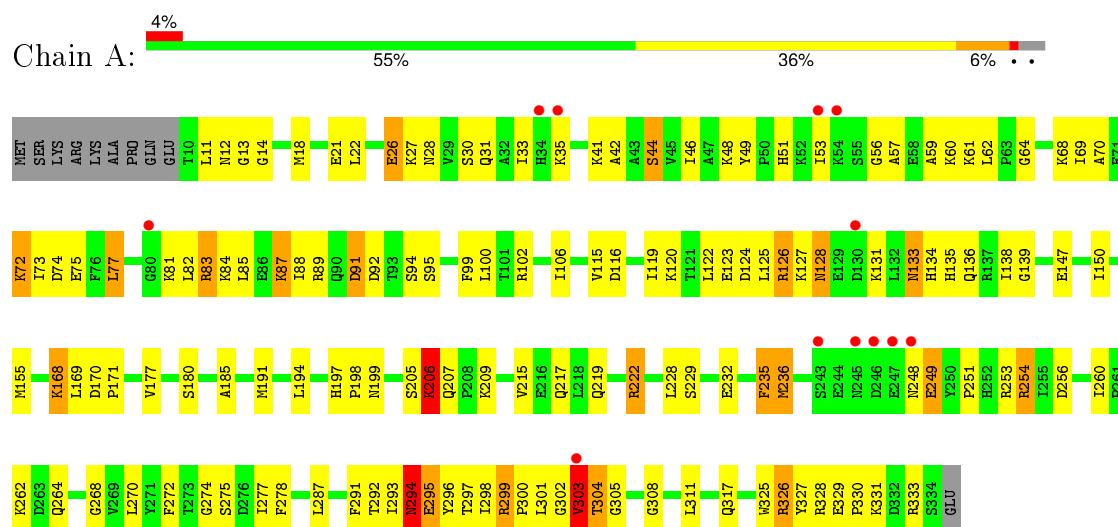
- Molecule 1: DNA polymerase beta

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.95Å 67.45Å 83.36Å 90.00° 116.14° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	83.9 (15.00-2.50) 83.8 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.14 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.250 , 0.317 0.238 , 0.305	Depositor DCC
R_{free} test set	1824 reflections (8.02%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.9	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 25239 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5379	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.67 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6824e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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	0.51	0/2658	0.68	1/3577 (0.0%)
1	B	0.43	0/2658	0.61	0/3577
All	All	0.47	0/5316	0.65	1/7154 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	294	ASN	N-CA-CB	-5.39	100.90	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	GLY	Peptide

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	2610	0	2629	132	0
1	B	2610	0	2629	181	0
2	A	95	0	0	6	0
2	B	64	0	0	14	0
All	All	5379	0	5258	313	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 30.

All (313) 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:264:GLN:HB2	1:A:296:TYR:O	1.62	0.99
1:A:12:ASN:HD21	1:A:53:ILE:H	1.12	0.94
1:B:197:HIS:HD2	1:B:199:ASN:H	1.15	0.92
1:B:62:LEU:H	1:B:62:LEU:HD12	1.32	0.92
1:A:294:ASN:HD22	1:A:296:TYR:H	1.16	0.91
1:B:69:ILE:H	1:B:69:ILE:HD12	1.37	0.89
1:B:119:ILE:HG22	1:B:125:LEU:HD23	1.52	0.89
1:A:294:ASN:ND2	1:A:296:TYR:H	1.71	0.89
1:A:134:HIS:CD2	1:A:138:ILE:HD11	2.08	0.88
1:B:22:LEU:HD11	1:B:85:LEU:HD11	1.55	0.87
1:A:168:LYS:HA	1:A:168:LYS:HE3	1.59	0.85
1:B:266:TYR:HA	1:B:269:VAL:HG22	1.59	0.83
1:B:87:LYS:HD2	1:B:87:LYS:C	2.00	0.82
1:A:197:HIS:HD2	1:A:199:ASN:H	1.30	0.80
1:A:197:HIS:CD2	1:A:199:ASN:H	1.99	0.80
1:B:205:SER:O	1:B:206:LYS:HB2	1.82	0.79
1:A:304:THR:HG22	1:A:305:GLY:H	1.47	0.79
1:B:75:GLU:HG2	1:B:82:LEU:HD12	1.65	0.78
1:B:283:ARG:HD3	2:B:389:HOH:O	1.82	0.78
1:A:18:MET:O	1:A:22:LEU:HD13	1.85	0.77
1:B:162:VAL:HB	2:B:349:HOH:O	1.85	0.76
1:A:150:ILE:HG21	1:A:155:MET:HE2	1.67	0.75
1:A:42:ALA:O	1:A:46:ILE:HD13	1.87	0.75
1:A:100:LEU:HD11	1:A:120:LYS:HA	1.67	0.75
1:B:197:HIS:CD2	1:B:199:ASN:H	2.03	0.75
1:B:115:VAL:HG13	1:B:120:LYS:HB3	1.69	0.74
1:A:133:ASN:HD22	1:A:133:ASN:C	1.90	0.74
1:B:244:GLU:O	1:B:245:ASN:HB3	1.87	0.74
1:B:105:GLY:HA3	1:B:136:GLN:HA	1.69	0.73
1:A:133:ASN:HD21	1:A:136:GLN:H	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LYS:H	1:B:89:ARG:HH21	1.37	0.73
1:B:183:ARG:NH1	2:B:354:HOH:O	2.22	0.73
1:B:29:VAL:O	1:B:29:VAL:HG12	1.89	0.72
1:B:275:SER:HB3	1:B:278:PHE:HB3	1.70	0.72
1:A:133:ASN:ND2	1:A:136:GLN:H	1.87	0.71
1:B:26:GLU:HA	1:B:30:SER:HB3	1.73	0.70
1:B:16:THR:O	1:B:20:VAL:HG12	1.91	0.70
1:B:56:GLY:HA2	1:B:59:ALA:HB3	1.73	0.70
1:B:62:LEU:N	1:B:62:LEU:HD12	2.05	0.69
1:B:186:GLU:OE1	1:B:187:SER:HB2	1.92	0.69
1:B:87:LYS:HD2	1:B:87:LYS:O	1.93	0.69
1:B:162:VAL:O	1:B:166:VAL:HG23	1.92	0.69
1:B:216:GLU:OE1	2:B:386:HOH:O	2.11	0.69
1:B:75:GLU:O	1:B:75:GLU:HG3	1.89	0.68
1:B:167:LYS:NZ	2:B:365:HOH:O	2.27	0.68
1:B:162:VAL:N	2:B:349:HOH:O	2.26	0.68
1:B:159:GLN:C	2:B:349:HOH:O	2.32	0.68
1:B:246:ASP:HB2	1:B:249:GLU:HB3	1.76	0.67
1:A:300:PRO:HD3	1:A:311:LEU:HD21	1.76	0.67
1:A:139:GLY:O	2:A:360:HOH:O	2.12	0.67
1:B:110:ALA:O	1:B:114:LEU:HD22	1.94	0.67
1:A:106:ILE:HG12	1:A:136:GLN:HG2	1.78	0.66
1:B:276:ASP:OD1	2:B:372:HOH:O	2.14	0.66
1:B:103:VAL:HG12	1:B:105:GLY:H	1.59	0.66
1:B:122:LEU:HD12	1:B:125:LEU:HD12	1.78	0.65
1:B:294:ASN:O	2:B:374:HOH:O	2.14	0.65
1:B:117:GLU:HG2	1:B:131:LYS:HE2	1.78	0.65
1:B:62:LEU:HD13	1:B:65:VAL:HG21	1.78	0.65
1:B:93:THR:HG22	1:B:112:ARG:NH2	2.12	0.65
1:A:69:ILE:O	1:A:73:ILE:HG13	1.98	0.64
1:A:12:ASN:O	1:A:14:GLY:N	2.29	0.64
1:A:294:ASN:HD21	1:A:296:TYR:HB2	1.62	0.64
1:B:106:ILE:HG12	1:B:136:GLN:NE2	2.12	0.64
1:B:299:ARG:HA	1:B:311:LEU:CD2	2.28	0.64
1:A:150:ILE:CD1	1:A:155:MET:HE3	2.27	0.64
1:A:125:LEU:C	1:A:127:LYS:H	2.02	0.63
1:B:87:LYS:HB2	1:B:90:GLN:CD	2.17	0.63
1:B:325:TRP:CE3	1:B:325:TRP:HA	2.33	0.63
1:A:294:ASN:HD22	1:A:296:TYR:N	1.92	0.62
1:A:205:SER:O	1:A:206:LYS:HB3	1.99	0.62
1:A:294:ASN:HD22	1:A:297:THR:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HH11	1:B:310:PRO:HG3	1.64	0.62
1:B:106:ILE:HG12	1:B:136:GLN:CD	2.20	0.62
1:B:201:THR:H	1:B:204:SER:HB2	1.63	0.62
1:B:113:LYS:HG3	1:B:114:LEU:HD13	1.81	0.61
1:B:36:TYR:HD2	1:B:37:ASN:ND2	1.98	0.61
1:A:72:LYS:O	1:A:75:GLU:HB3	1.99	0.61
1:A:56:GLY:HA2	1:A:59:ALA:HB3	1.82	0.61
1:B:93:THR:HG22	1:B:112:ARG:HH21	1.65	0.61
1:B:193:VAL:HG13	1:B:257:ILE:HG23	1.83	0.60
1:B:243:SER:HB3	1:B:249:GLU:HG3	1.83	0.60
1:B:247:GLU:O	1:B:248:ASN:HB2	2.02	0.60
1:A:30:SER:O	1:A:31:GLN:HB2	2.01	0.60
1:A:134:HIS:O	1:A:138:ILE:HD12	2.01	0.60
1:A:300:PRO:HD3	1:A:311:LEU:CD2	2.32	0.60
1:B:189:GLY:O	1:B:190:ASP:HB3	2.01	0.60
1:A:119:ILE:HG23	1:A:124:ASP:HB3	1.83	0.60
1:B:114:LEU:HD21	1:B:132:LEU:HD12	1.83	0.60
1:A:294:ASN:ND2	1:A:296:TYR:N	2.47	0.59
1:A:299:ARG:NH1	2:A:390:HOH:O	2.36	0.59
1:B:69:ILE:CD1	1:B:69:ILE:H	2.10	0.59
1:B:168:LYS:HB2	1:B:168:LYS:HZ3	1.68	0.58
1:B:125:LEU:C	1:B:127:LYS:H	2.07	0.58
1:B:325:TRP:HE3	1:B:325:TRP:HA	1.68	0.58
1:A:83:ARG:O	1:A:87:LYS:HE3	2.03	0.58
1:A:264:GLN:HA	2:A:397:HOH:O	2.03	0.58
1:A:198:PRO:HA	1:A:262:LYS:HG3	1.85	0.58
1:B:83:ARG:HA	1:B:86:GLU:HB2	1.85	0.58
1:A:133:ASN:H	1:A:136:GLN:NE2	2.02	0.58
1:A:205:SER:O	1:A:206:LYS:CB	2.51	0.58
1:B:330:PRO:O	1:B:333:ARG:HB2	2.04	0.58
1:A:304:THR:CG2	1:A:305:GLY:H	2.12	0.58
1:B:208:PRO:HB3	1:B:232:GLU:OE1	2.03	0.58
1:B:216:GLU:O	1:B:216:GLU:HG3	2.04	0.58
1:B:133:ASN:CG	1:B:137:ARG:HH12	2.06	0.58
1:A:304:THR:HG22	1:A:305:GLY:N	2.18	0.57
1:B:122:LEU:CD1	1:B:125:LEU:HD12	2.34	0.57
1:A:150:ILE:HG21	1:A:155:MET:CE	2.34	0.57
1:A:292:THR:OG1	1:A:301:LEU:HD12	2.04	0.57
1:A:235:PHE:C	1:A:235:PHE:CD2	2.77	0.56
1:B:174:ILE:HB	1:B:196:THR:HG22	1.87	0.56
1:A:177:VAL:CG1	1:A:191:MET:HG3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:O	1:B:29:VAL:CG1	2.53	0.56
1:B:276:ASP:HB2	2:B:372:HOH:O	2.06	0.56
1:B:243:SER:C	1:B:245:ASN:H	2.06	0.56
1:B:267:CYS:HB3	2:B:374:HOH:O	2.06	0.56
1:A:248:ASN:O	1:A:249:GLU:C	2.44	0.56
1:B:130:ASP:OD1	1:B:131:LYS:HG3	2.06	0.55
1:B:72:LYS:HB3	1:B:82:LEU:HD11	1.88	0.55
1:B:36:TYR:HD2	1:B:37:ASN:HD22	1.54	0.55
1:A:150:ILE:HD13	1:A:155:MET:CE	2.37	0.55
1:B:170:ASP:OD2	1:B:197:HIS:HE1	1.90	0.55
1:B:159:GLN:O	1:B:163:LEU:HB2	2.07	0.55
1:A:68:LYS:HG3	1:A:69:ILE:H	1.70	0.54
1:B:329:GLU:HG3	1:B:330:PRO:HD2	1.89	0.54
1:B:107:GLY:O	1:B:111:ALA:HB2	2.07	0.54
1:A:177:VAL:HG11	1:A:191:MET:HG3	1.89	0.54
1:B:82:LEU:HD23	1:B:84:LYS:HB3	1.87	0.54
1:A:100:LEU:HD22	1:A:115:VAL:HG23	1.89	0.54
1:B:294:ASN:HB3	1:B:296:TYR:H	1.72	0.54
1:B:202:SER:HB3	1:B:264:GLN:NE2	2.22	0.54
1:B:133:ASN:HB2	1:B:137:ARG:NH1	2.23	0.54
1:A:68:LYS:HG3	1:A:69:ILE:N	2.23	0.54
1:B:37:ASN:HD22	1:B:37:ASN:N	2.04	0.54
1:B:287:LEU:HD12	1:B:291:PHE:O	2.09	0.53
1:B:294:ASN:HB3	1:B:297:THR:H	1.73	0.53
1:A:81:LYS:HE2	1:A:89:ARG:NH2	2.24	0.53
1:B:134:HIS:H	1:B:137:ARG:NH2	2.07	0.53
1:A:91:ASP:N	1:A:91:ASP:OD2	2.41	0.53
1:A:236:MET:HB3	1:A:256:ASP:OD1	2.09	0.53
1:A:75:GLU:OE2	1:A:83:ARG:NE	2.42	0.52
1:A:197:HIS:HD2	1:A:199:ASN:N	2.03	0.52
1:B:104:THR:HG22	1:B:139:GLY:CA	2.39	0.52
1:B:251:PRO:HG2	1:B:253:ARG:CZ	2.38	0.52
1:B:104:THR:HG22	1:B:139:GLY:HA3	1.91	0.52
1:B:84:LYS:O	1:B:87:LYS:HG2	2.09	0.52
1:A:42:ALA:O	1:A:46:ILE:CD1	2.57	0.52
1:A:131:LYS:O	1:A:131:LYS:HD2	2.10	0.52
1:A:317:GLN:HE22	1:A:327:TYR:HB2	1.74	0.52
1:B:160:ASP:O	1:B:164:ASN:HB2	2.09	0.52
1:B:201:THR:HB	1:B:263:ASP:OD2	2.10	0.52
1:A:299:ARG:HG2	1:A:308:GLY:O	2.09	0.52
1:A:150:ILE:HD13	1:A:155:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:O	1:A:77:LEU:HD13	2.10	0.51
1:B:22:LEU:CD1	1:B:85:LEU:HD11	2.33	0.51
1:B:106:ILE:N	1:B:136:GLN:HG2	2.26	0.51
1:B:111:ALA:O	1:B:115:VAL:HG23	2.10	0.51
1:A:215:VAL:O	1:A:219:GLN:HG3	2.10	0.51
1:A:229:SER:HB3	1:A:236:MET:HG3	1.92	0.51
1:B:177:VAL:HG23	1:B:177:VAL:O	2.10	0.51
1:A:56:GLY:HA3	1:A:74:ASP:HB3	1.92	0.51
1:A:317:GLN:NE2	1:A:327:TYR:HB2	2.26	0.51
1:B:54:LYS:O	1:B:77:LEU:HD12	2.11	0.51
1:B:279:ASN:O	1:B:283:ARG:HG2	2.11	0.50
1:B:106:ILE:HD12	1:B:110:ALA:HB3	1.92	0.50
1:A:133:ASN:ND2	1:A:133:ASN:C	2.62	0.50
1:A:27:LYS:HG2	1:A:28:ASN:OD1	2.11	0.50
1:A:134:HIS:HD2	1:A:138:ILE:HD11	1.73	0.50
1:A:122:LEU:O	1:A:126:ARG:HG3	2.12	0.50
1:A:44:SER:O	1:A:48:LYS:HG2	2.11	0.50
1:A:60:LYS:HB2	1:A:70:ALA:HB1	1.94	0.49
1:B:75:GLU:HG2	1:B:82:LEU:CD1	2.39	0.49
1:B:159:GLN:O	1:B:159:GLN:HG2	2.10	0.49
1:B:244:GLU:O	1:B:245:ASN:CB	2.59	0.49
1:A:100:LEU:HD11	1:A:120:LYS:CA	2.39	0.49
1:B:159:GLN:HE21	1:B:177:VAL:HG22	1.78	0.49
1:B:106:ILE:HG23	1:B:110:ALA:HB3	1.94	0.49
1:B:311:LEU:N	1:B:311:LEU:HD22	2.27	0.49
1:A:82:LEU:HD12	1:A:83:ARG:N	2.28	0.49
1:B:170:ASP:OD1	1:B:171:PRO:HD2	2.12	0.49
1:B:113:LYS:HG3	1:B:114:LEU:CD1	2.43	0.49
1:B:274:GLY:O	1:B:275:SER:CB	2.60	0.49
1:B:329:GLU:HG2	1:B:331:LYS:NZ	2.28	0.49
1:A:287:LEU:HD23	1:A:291:PHE:O	2.13	0.49
1:A:302:GLY:O	1:A:303:VAL:C	2.51	0.48
1:B:132:LEU:HB3	1:B:136:GLN:HE22	1.76	0.48
1:B:186:GLU:CD	1:B:187:SER:HB2	2.32	0.48
1:B:93:THR:CG2	1:B:112:ARG:HH21	2.26	0.48
1:B:181:PHE:C	1:B:181:PHE:CD2	2.87	0.48
1:B:260:ILE:HG23	1:B:261:PRO:HD2	1.95	0.48
1:B:66:GLY:H	1:B:69:ILE:HD13	1.78	0.48
1:A:115:VAL:HG12	1:A:116:ASP:N	2.27	0.48
1:B:182:ARG:HD3	1:B:273:THR:OG1	2.13	0.48
1:B:269:VAL:HG23	1:B:270:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:O	1:A:311:LEU:HD23	2.14	0.47
1:B:133:ASN:HB2	1:B:134:HIS:H	1.46	0.47
1:A:197:HIS:CD2	1:A:199:ASN:HB2	2.49	0.47
1:B:297:THR:HB	1:B:310:PRO:HB3	1.95	0.47
1:B:122:LEU:HA	1:B:125:LEU:HD12	1.96	0.47
1:B:110:ALA:C	1:B:114:LEU:HD22	2.35	0.47
1:B:26:GLU:CA	1:B:30:SER:HB3	2.43	0.47
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.49	0.47
1:A:125:LEU:O	1:A:127:LYS:N	2.47	0.47
1:B:159:GLN:NE2	2:B:377:HOH:O	2.47	0.47
1:B:193:VAL:CG1	1:B:257:ILE:HG12	2.44	0.47
1:A:294:ASN:ND2	1:A:296:TYR:HB2	2.27	0.47
1:B:27:LYS:NZ	1:B:28:ASN:ND2	2.62	0.47
1:B:42:ALA:O	1:B:46:ILE:HG12	2.15	0.47
1:A:293:ILE:HG22	1:A:294:ASN:N	2.30	0.47
1:B:62:LEU:HD13	1:B:65:VAL:CG2	2.44	0.47
1:A:123:GLU:O	1:A:127:LYS:HE2	2.15	0.47
1:B:173:TYR:CD2	1:B:195:LEU:HD11	2.49	0.46
1:B:105:GLY:O	1:B:106:ILE:O	2.33	0.46
1:A:251:PRO:HG2	1:A:253:ARG:CZ	2.45	0.46
1:A:177:VAL:HG12	2:A:386:HOH:O	2.16	0.46
1:A:180:SER:O	1:A:185:ALA:HB3	2.15	0.46
1:B:87:LYS:C	1:B:89:ARG:N	2.67	0.46
1:A:26:GLU:O	1:A:30:SER:HB2	2.16	0.46
1:A:135:HIS:CD2	1:A:228:LEU:HB3	2.51	0.46
1:B:133:ASN:CB	1:B:137:ARG:NH1	2.79	0.46
1:B:116:ASP:C	1:B:118:GLY:N	2.70	0.46
1:A:294:ASN:ND2	1:A:297:THR:H	2.13	0.45
1:B:264:GLN:OE1	1:B:296:TYR:HB3	2.16	0.45
1:A:295:GLU:HG2	1:A:296:TYR:CD1	2.51	0.45
1:A:303:VAL:HG23	1:A:304:THR:H	1.81	0.45
1:B:276:ASP:O	1:B:280:LYS:HG2	2.16	0.45
1:B:267:CYS:CB	2:B:374:HOH:O	2.64	0.45
1:A:49:TYR:CE2	1:A:51:HIS:HB2	2.52	0.45
1:B:247:GLU:O	1:B:248:ASN:CB	2.65	0.45
1:A:41:LYS:HD3	1:A:41:LYS:HA	1.71	0.45
1:B:87:LYS:C	1:B:89:ARG:H	2.19	0.45
1:B:103:VAL:C	1:B:105:GLY:H	2.19	0.45
1:A:206:LYS:HB2	1:A:206:LYS:NZ	2.31	0.45
1:B:133:ASN:HB2	1:B:137:ARG:CZ	2.47	0.45
1:A:268:GLY:O	1:A:272:PHE:HD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HD11	1:B:77:LEU:HD21	1.98	0.45
1:B:313:VAL:CG2	1:B:313:VAL:O	2.65	0.45
1:B:209:LYS:O	1:B:213:ARG:HB2	2.16	0.45
1:B:299:ARG:HA	1:B:311:LEU:HD23	1.99	0.45
1:A:125:LEU:C	1:A:127:LYS:N	2.69	0.45
1:B:150:ILE:HG21	1:B:155:MET:SD	2.57	0.45
1:B:49:TYR:HA	1:B:50:PRO:HD2	1.85	0.44
1:A:53:ILE:HG22	1:A:77:LEU:HD21	1.99	0.44
1:B:99:PHE:CZ	1:B:122:LEU:HD22	2.52	0.44
1:A:294:ASN:HB3	1:A:297:THR:O	2.17	0.44
1:B:299:ARG:HB2	1:B:300:PRO:CD	2.47	0.44
1:A:219:GLN:O	1:A:222:ARG:NH1	2.51	0.44
1:B:107:GLY:O	1:B:111:ALA:CB	2.66	0.43
1:A:277:ILE:HA	1:A:277:ILE:HD13	1.81	0.43
1:A:84:LYS:NZ	2:A:376:HOH:O	2.50	0.43
1:B:87:LYS:HB2	1:B:90:GLN:NE2	2.31	0.43
1:B:311:LEU:HB3	1:B:312:PRO:HD2	2.00	0.43
1:A:135:HIS:CG	1:A:228:LEU:HB3	2.53	0.43
1:B:147:GLU:HG2	1:B:147:GLU:H	1.70	0.43
1:B:275:SER:HB3	1:B:278:PHE:CB	2.46	0.43
1:A:170:ASP:HA	1:A:171:PRO:HD3	1.77	0.43
1:B:246:ASP:CB	1:B:249:GLU:HB3	2.47	0.43
1:B:18:MET:O	1:B:22:LEU:HD12	2.19	0.43
1:B:276:ASP:CB	2:B:372:HOH:O	2.63	0.43
1:B:243:SER:C	1:B:245:ASN:N	2.73	0.42
1:A:264:GLN:HE21	1:A:264:GLN:HB3	1.68	0.42
1:B:133:ASN:O	1:B:135:HIS:CD2	2.72	0.42
1:A:169:LEU:HD21	1:A:217:GLN:HG2	2.01	0.42
1:A:91:ASP:O	1:A:92:ASP:C	2.57	0.42
1:A:12:ASN:ND2	1:A:53:ILE:H	1.96	0.42
1:A:68:LYS:HG3	1:A:69:ILE:HG13	2.02	0.42
1:B:125:LEU:C	1:B:127:LYS:N	2.72	0.42
1:A:254:ARG:NH2	1:A:256:ASP:OD1	2.53	0.42
1:A:68:LYS:HE3	1:A:69:ILE:HG13	2.02	0.42
1:B:249:GLU:O	1:B:250:TYR:C	2.57	0.42
1:B:208:PRO:CB	1:B:232:GLU:OE1	2.67	0.42
1:B:119:ILE:CG2	1:B:125:LEU:HD23	2.35	0.42
1:B:269:VAL:HG23	1:B:270:LEU:H	1.84	0.42
1:A:150:ILE:HG12	1:A:253:ARG:NE	2.35	0.42
1:A:328:ARG:O	1:A:329:GLU:C	2.55	0.42
1:A:106:ILE:CG1	1:A:136:GLN:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HB2	1:B:168:LYS:NZ	2.32	0.42
1:B:221:VAL:O	1:B:221:VAL:CG1	2.68	0.42
1:A:311:LEU:HD22	1:A:311:LEU:N	2.35	0.42
1:B:69:ILE:O	1:B:73:ILE:HG13	2.19	0.41
1:B:111:ALA:O	1:B:115:VAL:N	2.51	0.41
1:A:84:LYS:HE2	1:A:88:ILE:HD11	2.01	0.41
1:B:88:ILE:O	1:B:88:ILE:HG22	2.20	0.41
1:B:116:ASP:C	1:B:118:GLY:H	2.23	0.41
1:B:31:GLN:HA	1:B:31:GLN:NE2	2.36	0.41
1:B:138:ILE:HG21	1:B:228:LEU:HD21	2.02	0.41
1:A:21:GLU:HG3	2:A:399:HOH:O	2.20	0.41
1:B:216:GLU:O	1:B:216:GLU:CG	2.68	0.41
1:A:135:HIS:NE2	1:A:228:LEU:HD13	2.35	0.41
1:B:150:ILE:CG2	1:B:154:GLU:HB3	2.50	0.41
1:B:103:VAL:C	1:B:105:GLY:N	2.74	0.41
1:A:81:LYS:HE2	1:A:89:ARG:HH21	1.85	0.41
1:A:57:ALA:O	1:A:61:LYS:HG3	2.20	0.41
1:A:30:SER:O	1:A:31:GLN:CB	2.66	0.41
1:A:325:TRP:CD1	1:A:326:ARG:NH2	2.89	0.41
1:B:245:ASN:O	1:B:246:ASP:CG	2.59	0.41
1:B:105:GLY:HA3	1:B:136:GLN:CA	2.43	0.41
1:A:33:ILE:HD12	1:A:33:ILE:N	2.35	0.41
1:B:197:HIS:CD2	1:B:199:ASN:HB2	2.56	0.41
1:B:26:GLU:HG3	1:B:39:TYR:HE1	1.85	0.41
1:A:150:ILE:HB	1:A:155:MET:HE3	2.02	0.41
1:B:209:LYS:O	1:B:209:LYS:HD3	2.21	0.41
1:A:278:PHE:CE2	1:A:333:ARG:HD3	2.55	0.41
1:B:19:LEU:HB3	1:B:43:ALA:HB2	2.03	0.40
1:A:53:ILE:HD12	1:A:59:ALA:HB2	2.03	0.40
1:A:150:ILE:HD12	1:A:155:MET:HE3	2.03	0.40
1:A:329:GLU:HA	1:A:330:PRO:HD3	1.94	0.40
1:A:99:PHE:O	1:A:102:ARG:HG2	2.20	0.40
1:B:99:PHE:HE2	1:B:122:LEU:HB2	1.87	0.40
1:B:313:VAL:HG22	1:B:313:VAL:O	2.21	0.40
1:B:121:THR:OG1	1:B:122:LEU:N	2.54	0.40
1:A:150:ILE:HG12	1:A:253:ARG:CZ	2.52	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.63	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	323/335 (96%)	275 (85%)	36 (11%)	12 (4%)	4	5
1	B	323/335 (96%)	271 (84%)	31 (10%)	21 (6%)	1	1
All	All	646/670 (96%)	546 (84%)	67 (10%)	33 (5%)	2	2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	206	LYS
1	A	249	GLU
1	A	303	VAL
1	B	87	LYS
1	B	106	ILE
1	B	204	SER
1	B	205	SER
1	B	245	ASN
1	B	248	ASN
1	B	250	TYR
1	B	275	SER
1	A	13	GLY
1	A	95	SER
1	A	126	ARG
1	B	108	PRO
1	B	121	THR
1	B	130	ASP
1	B	133	ASN
1	B	134	HIS
1	B	206	LYS
1	B	274	GLY
1	A	94	SER
1	A	275	SER
1	A	304	THR

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Mol	Chain	Res	Type
1	B	61	LYS
1	B	86	GLU
1	B	126	ARG
1	B	129	GLU
1	B	132	LEU
1	B	190	ASP
1	A	11	LEU
1	A	64	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	286/296 (97%)	256 (90%)	30 (10%)	8	16
1	B	286/296 (97%)	242 (85%)	44 (15%)	3	6
All	All	572/592 (97%)	498 (87%)	74 (13%)	5	10

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	35	LYS
1	A	44	SER
1	A	62	LEU
1	A	72	LYS
1	A	77	LEU
1	A	83	ARG
1	A	87	LYS
1	A	91	ASP
1	A	128	ASN
1	A	133	ASN
1	A	147	GLU
1	A	168	LYS
1	A	194	LEU
1	A	206	LYS

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Mol	Chain	Res	Type
1	A	207	GLN
1	A	209	LYS
1	A	222	ARG
1	A	232	GLU
1	A	235	PHE
1	A	236	MET
1	A	254	ARG
1	A	260	ILE
1	A	270	LEU
1	A	294	ASN
1	A	295	GLU
1	A	299	ARG
1	A	303	VAL
1	A	326	ARG
1	A	331	LYS
1	B	19	LEU
1	B	21	GLU
1	B	33	ILE
1	B	34	HIS
1	B	45	VAL
1	B	62	LEU
1	B	69	ILE
1	B	71	GLU
1	B	75	GLU
1	B	77	LEU
1	B	82	LEU
1	B	83	ARG
1	B	87	LYS
1	B	89	ARG
1	B	91	ASP
1	B	92	ASP
1	B	113	LYS
1	B	114	LEU
1	B	119	ILE
1	B	133	ASN
1	B	135	HIS
1	B	136	GLN
1	B	147	GLU
1	B	154	GLU
1	B	168	LYS
1	B	169	LEU
1	B	186	GLU

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Mol	Chain	Res	Type
1	B	187	SER
1	B	199	ASN
1	B	205	SER
1	B	206	LYS
1	B	233	THR
1	B	260	ILE
1	B	263	ASP
1	B	288	GLU
1	B	292	THR
1	B	303	VAL
1	B	304	THR
1	B	306	VAL
1	B	317	GLN
1	B	325	TRP
1	B	329	GLU
1	B	331	LYS
1	B	334	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	98	ASN
1	A	128	ASN
1	A	133	ASN
1	A	136	GLN
1	A	197	HIS
1	A	248	ASN
1	A	252	HIS
1	A	264	GLN
1	A	294	ASN
1	A	317	GLN
1	A	324	GLN
1	B	28	ASN
1	B	31	GLN
1	B	37	ASN
1	B	134	HIS
1	B	135	HIS
1	B	136	GLN
1	B	159	GLN
1	B	197	HIS
1	B	199	ASN

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Mol	Chain	Res	Type
1	B	240	GLN
1	B	317	GLN

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	325/335 (97%)	0.05	12 (3%)	45	50	13, 30, 70, 92	0
1	B	325/335 (97%)	0.34	22 (6%)	20	23	24, 42, 93, 105	0
All	All	650/670 (97%)	0.20	34 (5%)	31	35	13, 38, 86, 105	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ASP	7.2
1	A	248	ASN	6.3
1	B	119	ILE	5.7
1	B	248	ASN	5.2
1	A	247	GLU	4.7
1	B	132	LEU	4.1
1	A	245	ASN	4.0
1	B	107	GLY	4.0
1	B	92	ASP	3.7
1	B	120	LYS	3.7
1	B	94	SER	3.5
1	A	303	VAL	3.2
1	B	114	LEU	2.9
1	A	130	ASP	2.7
1	A	54	LYS	2.7
1	A	243	SER	2.7
1	A	35	LYS	2.6
1	B	109	SER	2.6
1	B	135	HIS	2.5
1	B	91	ASP	2.4
1	B	80	GLY	2.3
1	A	53	ILE	2.3
1	B	130	ASP	2.3
1	B	106	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	80	GLY	2.3
1	B	93	THR	2.2
1	B	89	ARG	2.2
1	B	69	ILE	2.2
1	B	67	THR	2.1
1	B	118	GLY	2.1
1	A	34	HIS	2.1
1	B	116	ASP	2.1
1	B	115	VAL	2.0
1	B	205	SER	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.