Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:13 am BST

PDB ID	:	3CDI
Title	:	Crystal structure of E. coli PNPase
Authors	:	Shi, Z.; Yang, W.Z.; Lin-Chao, S.; Chak, K.F.; Yuan, H.S.
Deposited on	:	2008-02-27
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:

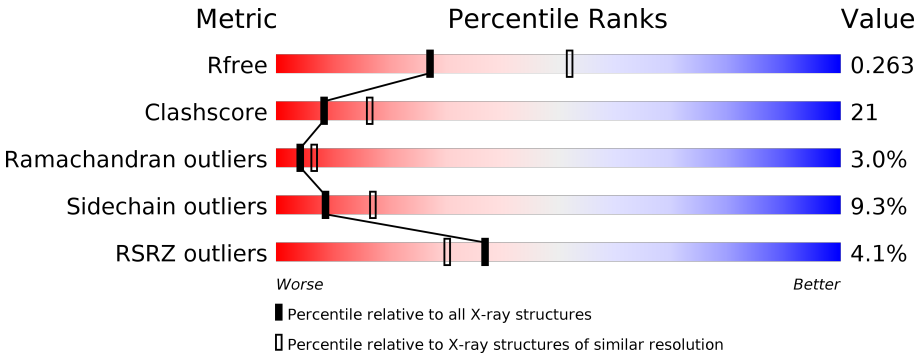
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	723	3% 43% 25% . 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4025 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 Polynucleotide phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	3924	2462	684	759	19	0	0	0

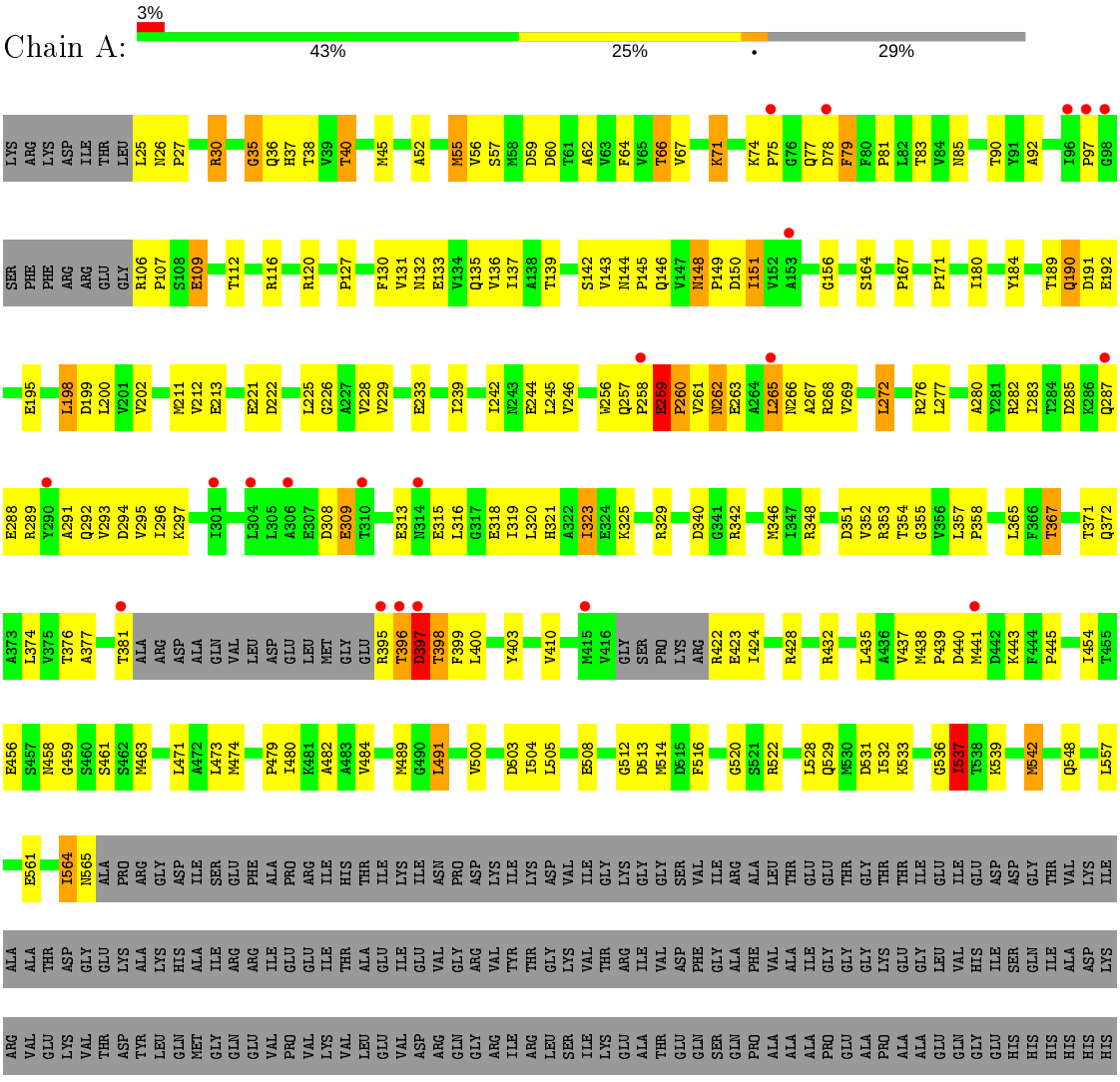
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	101	101	101	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: Polynucleotide phosphorylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	270.12Å 270.12Å 270.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 35.17 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.0 (50.00-2.60) 99.3 (35.17-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.58 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.277 0.255 , 0.263	Depositor DCC
R_{free} test set	2644 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4025	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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	0.37	0/3980	0.66	1/5393 (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	397	ASP	N-CA-C	-5.60	95.87	111.00

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	3924	0	3955	164	0
2	A	101	0	0	5	0
All	All	4025	0	3955	164	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 (164) 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:106:ARG:HB3	1:A:107:PRO:HA	1.25	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:HG3	1:A:189:THR:HB	1.42	1.00
1:A:171:PRO:HG2	1:A:239:ILE:HG23	1.45	0.99
1:A:396:THR:O	1:A:397:ASP:HB3	1.62	0.97
1:A:106:ARG:HB3	1:A:107:PRO:CA	1.98	0.92
1:A:437:VAL:HG12	1:A:480:ILE:HB	1.52	0.90
1:A:77:GLN:HB3	1:A:131:VAL:HG11	1.57	0.86
1:A:109:GLU:HB2	1:A:424:ILE:HD11	1.58	0.85
1:A:309:GLU:HB2	2:A:817:HOH:O	1.76	0.83
1:A:40:THR:HG23	1:A:57:SER:HB3	1.60	0.81
1:A:557:LEU:O	1:A:561:GLU:HG3	1.80	0.79
1:A:202:VAL:HG12	1:A:212:VAL:HG22	1.64	0.79
1:A:283:ILE:HD11	1:A:289:ARG:HA	1.67	0.77
1:A:66:THR:HG23	2:A:763:HOH:O	1.86	0.75
1:A:372:GLN:HB3	1:A:456:GLU:HB2	1.67	0.74
1:A:294:ASP:HB3	2:A:835:HOH:O	1.87	0.74
1:A:148:ASN:ND2	1:A:150:ASP:H	1.85	0.73
1:A:348:ARG:HD3	1:A:503:ASP:OD1	1.89	0.72
1:A:320:LEU:O	1:A:323:ILE:HD13	1.88	0.72
1:A:148:ASN:HD22	1:A:149:PRO:N	1.88	0.72
1:A:437:VAL:CG1	1:A:480:ILE:HB	2.19	0.71
1:A:74:LYS:HB3	1:A:75:PRO:HD2	1.75	0.69
1:A:258:PRO:O	1:A:259:GLU:HB3	1.91	0.68
1:A:308:ASP:CG	1:A:309:GLU:H	1.95	0.67
1:A:403:TYR:OH	1:A:461:SER:HB2	1.95	0.67
1:A:437:VAL:HG13	1:A:482:ALA:H	1.60	0.66
1:A:351:ASP:HB3	1:A:367:THR:HG23	1.77	0.66
1:A:513:ASP:HA	1:A:533:LYS:HE2	1.77	0.66
1:A:285:ASP:HB2	1:A:288:GLU:HB3	1.79	0.65
1:A:410:VAL:O	1:A:410:VAL:HG12	1.97	0.65
1:A:198:LEU:HD22	1:A:199:ASP:N	2.10	0.64
1:A:30:ARG:HH21	1:A:244:GLU:HG3	1.62	0.64
1:A:200:LEU:HD21	1:A:202:VAL:HG13	1.80	0.63
1:A:59:ASP:O	1:A:60:ASP:HB2	1.97	0.63
1:A:40:THR:CG2	1:A:57:SER:HB3	2.27	0.63
1:A:522:ARG:NH1	1:A:561:GLU:OE1	2.32	0.62
1:A:81:PRO:HB2	1:A:133:GLU:HG3	1.83	0.61
1:A:489:MET:HB2	1:A:516:PHE:CE2	2.36	0.61
1:A:537:ILE:O	1:A:537:ILE:HD13	2.01	0.61
1:A:131:VAL:HG12	1:A:131:VAL:O	2.01	0.60
1:A:280:ALA:O	1:A:283:ILE:HG12	2.00	0.60
1:A:438:MET:HE1	1:A:473:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:O	1:A:272:LEU:HD21	2.02	0.60
1:A:37:HIS:HD2	1:A:59:ASP:OD2	1.86	0.59
1:A:148:ASN:HD22	1:A:148:ASN:C	2.05	0.59
1:A:242:ILE:O	1:A:246:VAL:HG23	2.02	0.59
1:A:92:ALA:HB1	1:A:143:VAL:HG23	1.85	0.59
1:A:35:GLY:O	1:A:36:GLN:HB3	2.03	0.59
1:A:74:LYS:HB2	1:A:77:GLN:HG2	1.83	0.59
1:A:537:ILE:C	1:A:537:ILE:HD13	2.23	0.58
1:A:291:ALA:O	1:A:295:VAL:HG23	2.02	0.58
1:A:395:ARG:HG2	1:A:398:THR:CG2	2.33	0.58
1:A:55:MET:HG2	1:A:64:PHE:CD1	2.38	0.58
1:A:256:TRP:CZ2	1:A:258:PRO:HA	2.39	0.58
1:A:395:ARG:HD3	1:A:399:PHE:HB2	1.86	0.57
1:A:463:MET:HA	1:A:463:MET:CE	2.34	0.57
1:A:150:ASP:OD1	1:A:151:ILE:N	2.37	0.57
1:A:340:ASP:OD1	1:A:342:ARG:HD3	2.04	0.57
1:A:148:ASN:HD22	1:A:150:ASP:H	1.51	0.55
1:A:491:LEU:HB3	1:A:514:MET:HB3	1.87	0.55
1:A:537:ILE:O	1:A:537:ILE:HG23	2.07	0.55
1:A:463:MET:HE2	1:A:463:MET:HA	1.88	0.55
1:A:395:ARG:NH1	1:A:439:PRO:O	2.41	0.54
1:A:308:ASP:CG	1:A:309:GLU:N	2.60	0.54
1:A:422:ARG:NE	1:A:422:ARG:HA	2.22	0.54
1:A:30:ARG:NH2	1:A:244:GLU:HG3	2.23	0.54
1:A:77:GLN:O	1:A:78:ASP:HB2	2.07	0.54
1:A:277:LEU:HD12	1:A:323:ILE:HD11	1.91	0.53
1:A:55:MET:HG2	1:A:64:PHE:HD1	1.74	0.53
1:A:395:ARG:O	1:A:396:THR:O	2.27	0.53
1:A:79:PHE:O	1:A:131:VAL:HG13	2.09	0.52
1:A:256:TRP:CH2	1:A:258:PRO:HA	2.45	0.52
1:A:321:HIS:NE2	1:A:325:LYS:HE2	2.25	0.52
1:A:308:ASP:O	1:A:309:GLU:HB3	2.09	0.52
1:A:441:MET:HE3	1:A:445:PRO:HA	1.92	0.52
1:A:292:GLN:O	1:A:296:ILE:HG13	2.10	0.51
1:A:259:GLU:HG3	1:A:259:GLU:O	2.11	0.51
1:A:225:LEU:HD21	1:A:542:MET:HB3	1.91	0.51
1:A:202:VAL:HG11	1:A:228:VAL:HA	1.92	0.51
1:A:229:VAL:O	1:A:233:GLU:HG3	2.11	0.51
1:A:354:THR:CG2	1:A:355:GLY:N	2.73	0.51
1:A:500:VAL:HB	1:A:548:GLN:NE2	2.26	0.51
1:A:79:PHE:C	1:A:131:VAL:HG13	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HH21	1:A:296:ILE:HA	1.76	0.50
1:A:396:THR:C	1:A:398:THR:H	2.11	0.50
1:A:120:ARG:NH2	1:A:213:GLU:HB2	2.26	0.50
1:A:27:PRO:HB3	1:A:45:MET:HB2	1.92	0.50
1:A:329:ARG:NH2	1:A:513:ASP:OD1	2.44	0.50
1:A:376:THR:HG22	1:A:377:ALA:N	2.27	0.50
1:A:352:VAL:HG13	1:A:471:LEU:HD13	1.93	0.50
1:A:272:LEU:N	1:A:272:LEU:HD23	2.26	0.50
1:A:474:MET:SD	1:A:564:ILE:HD12	2.51	0.50
1:A:190:GLN:HG3	1:A:191:ASP:N	2.26	0.50
1:A:90:THR:OG1	1:A:97:PRO:HD3	2.12	0.49
1:A:283:ILE:CD1	1:A:289:ARG:HA	2.40	0.49
1:A:395:ARG:HG2	1:A:398:THR:HG22	1.94	0.49
1:A:30:ARG:HH21	1:A:244:GLU:CG	2.25	0.49
1:A:213:GLU:OE1	1:A:529:GLN:HG3	2.13	0.49
1:A:130:PHE:CZ	1:A:132:ASN:HB2	2.48	0.49
1:A:351:ASP:OD2	1:A:353:ARG:NH1	2.47	0.48
1:A:258:PRO:O	1:A:259:GLU:CB	2.59	0.47
1:A:261:VAL:O	1:A:263:GLU:N	2.46	0.47
1:A:277:LEU:CD1	1:A:323:ILE:HD11	2.45	0.47
1:A:484:VAL:HG23	1:A:520:GLY:C	2.35	0.47
1:A:56:VAL:HG21	1:A:156:GLY:HA2	1.97	0.47
1:A:285:ASP:CB	1:A:288:GLU:HB3	2.45	0.47
1:A:85:ASN:ND2	1:A:135:GLN:HE21	2.13	0.47
1:A:536:GLY:O	1:A:537:ILE:C	2.51	0.47
1:A:308:ASP:O	1:A:309:GLU:CB	2.63	0.46
1:A:381:THR:O	1:A:381:THR:HG22	2.15	0.46
1:A:397:ASP:OD2	1:A:397:ASP:C	2.54	0.46
1:A:79:PHE:O	1:A:81:PRO:HD3	2.16	0.46
1:A:432:ARG:HA	1:A:435:LEU:HD12	1.97	0.46
1:A:342:ARG:NH2	1:A:503:ASP:HB3	2.30	0.46
1:A:438:MET:CE	1:A:473:LEU:HD13	2.46	0.46
1:A:66:THR:HG22	1:A:137:ILE:HB	1.97	0.46
1:A:55:MET:HE1	1:A:62:ALA:HB1	1.98	0.45
1:A:422:ARG:O	1:A:424:ILE:N	2.49	0.45
1:A:266:ASN:HB3	1:A:319:ILE:HD13	1.99	0.45
1:A:422:ARG:NE	1:A:422:ARG:CA	2.79	0.45
1:A:395:ARG:HG2	1:A:398:THR:HG21	1.98	0.45
1:A:92:ALA:CB	1:A:143:VAL:HG23	2.47	0.45
1:A:120:ARG:HH22	1:A:213:GLU:HB2	1.82	0.45
1:A:297:LYS:HG2	1:A:320:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLU:O	1:A:318:GLU:HB3	2.18	0.44
1:A:422:ARG:C	1:A:424:ILE:H	2.21	0.44
1:A:441:MET:CE	1:A:445:PRO:HA	2.47	0.44
1:A:30:ARG:HB2	1:A:245:LEU:HD13	1.99	0.44
1:A:25:LEU:HG	1:A:45:MET:HG3	1.98	0.44
1:A:144:ASN:O	1:A:146:GLN:N	2.51	0.44
1:A:454:ILE:HG13	1:A:461:SER:HB3	1.99	0.44
1:A:180:ILE:HG12	1:A:195:GLU:O	2.18	0.44
1:A:564:ILE:O	1:A:565:ASN:C	2.55	0.44
1:A:342:ARG:HB3	1:A:346:MET:HB2	2.01	0.43
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.84	0.43
1:A:71:LYS:HG2	2:A:833:HOH:O	2.17	0.43
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.85	0.43
1:A:30:ARG:HG2	2:A:830:HOH:O	2.17	0.43
1:A:52:ALA:HB2	1:A:164:SER:HA	2.01	0.43
1:A:265:LEU:O	1:A:269:VAL:HG23	2.19	0.42
1:A:313:GLU:O	1:A:316:LEU:HB2	2.19	0.42
1:A:443:LYS:HE2	1:A:479:PRO:HB2	2.02	0.42
1:A:357:LEU:HA	1:A:358:PRO:HD3	1.75	0.42
1:A:67:VAL:HG22	1:A:136:VAL:HG22	2.01	0.42
1:A:148:ASN:HA	1:A:149:PRO:HD3	1.90	0.42
1:A:189:THR:HG23	1:A:192:GLU:OE1	2.20	0.42
1:A:340:ASP:OD1	1:A:342:ARG:CD	2.67	0.42
1:A:428:ARG:O	1:A:432:ARG:HG3	2.20	0.42
1:A:289:ARG:O	1:A:293:VAL:HG23	2.20	0.41
1:A:505:LEU:HB2	1:A:508:GLU:HG3	2.01	0.41
1:A:265:LEU:C	1:A:267:ALA:H	2.23	0.41
1:A:395:ARG:O	1:A:396:THR:C	2.59	0.41
1:A:184:TYR:OH	1:A:226:GLY:HA3	2.21	0.41
1:A:120:ARG:NH1	1:A:531:ASP:OD2	2.51	0.41
1:A:512:GLY:C	1:A:514:MET:N	2.73	0.41
1:A:62:ALA:HB3	1:A:142:SER:OG	2.20	0.41
1:A:437:VAL:HG12	1:A:437:VAL:O	2.20	0.41
1:A:127:PRO:HD2	1:A:167:PRO:O	2.21	0.40
1:A:532:ILE:N	1:A:532:ILE:HD12	2.35	0.40
1:A:106:ARG:CB	1:A:107:PRO:CA	2.83	0.40
1:A:277:LEU:HD23	1:A:296:ILE:HD12	2.03	0.40
1:A:148:ASN:HD22	1:A:149:PRO:CD	2.34	0.40
1:A:262:ASN:OD1	1:A:265:LEU:HB2	2.22	0.40
1:A:78:ASP:O	1:A:79:PHE:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	508/723 (70%)	454 (89%)	39 (8%)	15 (3%)	4 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	THR
1	A	423	GLU
1	A	537	ILE
1	A	35	GLY
1	A	260	PRO
1	A	309	GLU
1	A	458	ASN
1	A	397	ASP
1	A	257	GLN
1	A	259	GLU
1	A	262	ASN
1	A	440	ASP
1	A	145	PRO
1	A	79	PHE
1	A	459	GLY

5.3.2 Protein sidechains

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	420/587 (72%)	381 (91%)	39 (9%)	9 17

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	30	ARG
1	A	38	THR
1	A	40	THR
1	A	55	MET
1	A	66	THR
1	A	71	LYS
1	A	83	THR
1	A	109	GLU
1	A	112	THR
1	A	116	ARG
1	A	139	THR
1	A	148	ASN
1	A	151	ILE
1	A	190	GLN
1	A	198	LEU
1	A	211	MET
1	A	221	GLU
1	A	222	ASP
1	A	259	GLU
1	A	260	PRO
1	A	265	LEU
1	A	272	LEU
1	A	287	GLN
1	A	323	ILE
1	A	365	LEU
1	A	367	THR
1	A	371	THR
1	A	374	LEU
1	A	397	ASP
1	A	398	THR
1	A	400	LEU
1	A	491	LEU
1	A	504	ILE
1	A	528	LEU
1	A	537	ILE
1	A	539	LYS
1	A	542	MET
1	A	564	ILE

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	33	GLN
1	A	37	HIS
1	A	85	ASN
1	A	146	GLN
1	A	148	ASN
1	A	257	GLN
1	A	266	ASN
1	A	287	GLN
1	A	426	HIS
1	A	510	HIS
1	A	543	GLN
1	A	548	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	516/723 (71%)	0.24	21 (4%) 37 30	27, 49, 88, 97	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	GLN	4.2
1	A	75	PRO	3.7
1	A	395	ARG	3.5
1	A	98	GLY	3.1
1	A	396	THR	2.9
1	A	314	ASN	2.9
1	A	415	MET	2.7
1	A	397	ASP	2.6
1	A	258	PRO	2.5
1	A	153	ALA	2.5
1	A	290	TYR	2.5
1	A	441	MET	2.4
1	A	78	ASP	2.3
1	A	381	THR	2.3
1	A	96	ILE	2.3
1	A	301	ILE	2.2
1	A	306	ALA	2.2
1	A	265	LEU	2.1
1	A	310	THR	2.1
1	A	97	PRO	2.0
1	A	304	LEU	2.0

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.