Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 AM GMT

PDB ID	:	2ZXO
Title	:	Crystal structure of RecJ from Thermus thermophilus HB8
Authors	:	Wakamatsu, T.; Kitamura, Y.; Nakagawa, N.; Masui, R.; Kuramitsu, S.
Deposited on	:	2009-01-05
Resolution	:	2.50 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 ⓘ symbol.

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

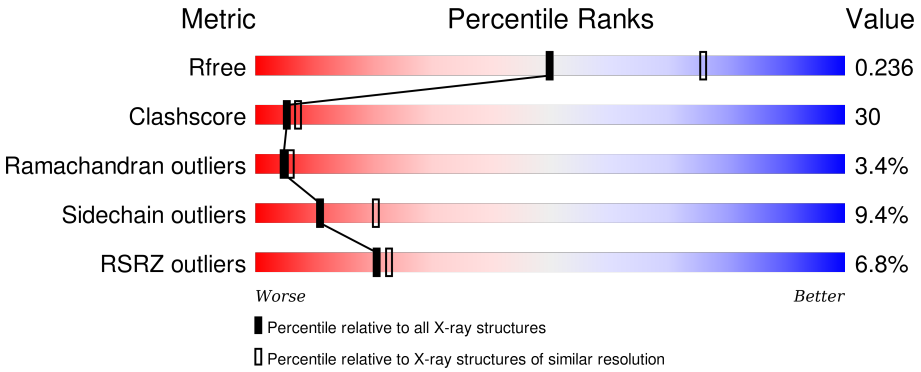
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	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	666	7%, 57%, 33%, 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5200 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 Single-stranded DNA specific exonuclease RecJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	648	5020	3230	903	880	7	0	0	0

- Molecule 2 is water.

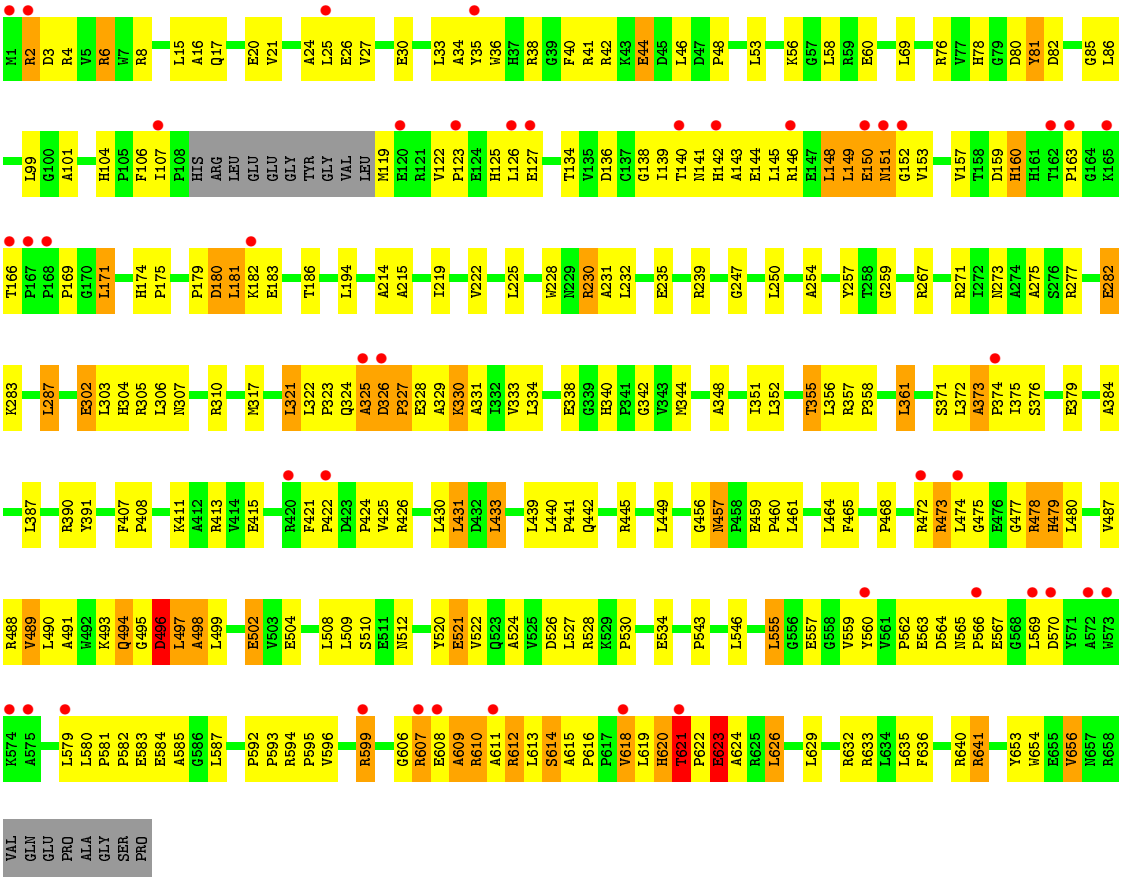
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	180	180	180	0	0

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: Single-stranded DNA specific exonuclease RecJ

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	82.98Å 82.98Å 249.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.72 – 2.50 49.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.72-2.50) 99.9 (49.83-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.64 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.282 0.238 , 0.236	Depositor DCC
R_{free} test set	1567 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 31195 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5200	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.56	0/5145	0.77	2/7012 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	614	SER	N-CA-C	-5.29	96.70	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	5020	0	5130	306	0
2	A	180	0	0	16	0
All	All	5200	0	5130	306	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 (306) 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:621:THR:HG23	1:A:622:PRO:HD3	1.31	1.09
1:A:138:GLY:HA2	1:A:141:ASN:HD22	1.22	1.05
1:A:433:LEU:HD23	1:A:632:ARG:HG2	1.43	0.99
1:A:614:SER:HB2	1:A:635:LEU:HD21	1.41	0.98
1:A:69:LEU:HD11	1:A:101:ALA:HB2	1.45	0.97
1:A:565:ASN:HD21	1:A:567:GLU:HB3	1.29	0.96
1:A:478:ARG:HH12	1:A:495:GLY:HA2	1.30	0.95
1:A:565:ASN:ND2	1:A:567:GLU:HB3	1.80	0.94
1:A:457:ASN:HD22	1:A:457:ASN:N	1.64	0.93
1:A:326:ASP:H	1:A:327:PRO:HD2	1.31	0.93
1:A:326:ASP:N	1:A:327:PRO:HD2	1.82	0.92
1:A:581:PRO:HG2	1:A:584:GLU:HG2	1.50	0.92
1:A:457:ASN:HD22	1:A:457:ASN:H	0.89	0.89
1:A:596:VAL:HG12	1:A:599:ARG:HG3	1.52	0.89
1:A:560:TYR:CE2	1:A:582:PRO:HD3	2.07	0.89
1:A:373:ALA:HB1	1:A:374:PRO:CD	2.02	0.88
1:A:384:ALA:HB2	1:A:413:ARG:HG2	1.54	0.88
1:A:457:ASN:ND2	1:A:457:ASN:H	1.74	0.85
1:A:6:ARG:HD2	1:A:425:VAL:HG21	1.58	0.85
1:A:546:LEU:HD22	1:A:606:GLY:HA2	1.59	0.84
1:A:76:ARG:HE	1:A:104:HIS:HE1	1.24	0.84
1:A:81:TYR:HB3	1:A:107:ILE:HD11	1.58	0.83
1:A:126:LEU:HD21	1:A:151:ASN:HB3	1.60	0.81
1:A:145:LEU:HA	2:A:825:HOH:O	1.80	0.81
1:A:138:GLY:HA2	1:A:141:ASN:ND2	1.95	0.81
1:A:329:ALA:O	1:A:331:ALA:N	2.12	0.80
1:A:592:PRO:HG2	1:A:654:TRP:CH2	2.16	0.80
1:A:76:ARG:HH11	1:A:125:HIS:HD2	1.30	0.79
1:A:592:PRO:HG2	1:A:654:TRP:HH2	1.47	0.79
1:A:340:HIS:HD2	1:A:342:GLY:H	1.30	0.79
1:A:614:SER:HB2	1:A:635:LEU:CD2	2.13	0.79
1:A:599:ARG:HA	2:A:779:HOH:O	1.83	0.78
1:A:559:VAL:HG12	1:A:587:LEU:HD23	1.67	0.77
1:A:324:GLN:O	1:A:326:ASP:OD1	2.05	0.75
1:A:592:PRO:O	1:A:654:TRP:HZ3	1.68	0.75
1:A:328:GLU:HA	2:A:835:HOH:O	1.85	0.75
1:A:478:ARG:NH1	1:A:495:GLY:HA2	2.02	0.75
1:A:562:PRO:HG2	2:A:845:HOH:O	1.87	0.74
1:A:474:LEU:HD12	2:A:840:HOH:O	1.87	0.74
1:A:621:THR:CG2	1:A:622:PRO:HD3	2.16	0.74
1:A:566:PRO:HA	1:A:569:LEU:HB3	1.68	0.74
1:A:473:ARG:HD3	1:A:475:GLY:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.52	0.73
1:A:433:LEU:HD23	1:A:632:ARG:CG	2.16	0.73
1:A:60:GLU:CD	1:A:171:LEU:HD21	2.09	0.73
1:A:565:ASN:ND2	1:A:610:ARG:HG3	2.04	0.73
1:A:442:GLN:NE2	1:A:445:ARG:HH21	1.86	0.72
1:A:2:ARG:HH21	1:A:3:ASP:HB3	1.52	0.72
1:A:442:GLN:HE21	1:A:445:ARG:HH21	1.37	0.72
1:A:478:ARG:HH12	1:A:495:GLY:CA	2.02	0.72
1:A:373:ALA:CB	1:A:374:PRO:CD	2.67	0.71
1:A:46:LEU:O	1:A:230:ARG:NH1	2.23	0.71
1:A:2:ARG:HH21	1:A:3:ASP:CB	2.03	0.71
1:A:81:TYR:CB	1:A:107:ILE:HD11	2.21	0.70
1:A:327:PRO:O	2:A:835:HOH:O	2.07	0.70
1:A:546:LEU:HD22	1:A:606:GLY:CA	2.21	0.70
1:A:623:GLU:O	1:A:623:GLU:HG3	1.92	0.70
1:A:76:ARG:NH1	1:A:125:HIS:HD2	1.89	0.69
1:A:16:ALA:O	1:A:20:GLU:HG3	1.93	0.68
1:A:384:ALA:HB2	1:A:413:ARG:CG	2.23	0.68
1:A:592:PRO:O	1:A:654:TRP:CZ3	2.45	0.67
1:A:384:ALA:CB	1:A:413:ARG:HG2	2.24	0.67
1:A:17:GLN:NE2	1:A:36:TRP:HE1	1.92	0.67
1:A:546:LEU:HD13	1:A:606:GLY:HA2	1.77	0.67
1:A:76:ARG:HH11	1:A:125:HIS:CD2	2.12	0.67
1:A:373:ALA:HB1	1:A:374:PRO:HD2	1.75	0.66
1:A:3:ASP:OD2	1:A:3:ASP:O	2.14	0.66
1:A:143:ALA:C	1:A:145:LEU:H	1.99	0.66
1:A:622:PRO:C	1:A:624:ALA:H	1.98	0.66
1:A:632:ARG:HD2	2:A:812:HOH:O	1.94	0.66
1:A:17:GLN:HE21	1:A:36:TRP:HE1	1.42	0.66
1:A:583:GLU:O	1:A:599:ARG:HD2	1.95	0.65
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.26	0.65
1:A:609:ALA:HB1	2:A:778:HOH:O	1.95	0.65
1:A:411:LYS:O	1:A:415:GLU:HG3	1.96	0.65
1:A:282:GLU:H	1:A:282:GLU:CD	2.01	0.64
1:A:583:GLU:HA	1:A:599:ARG:HD2	1.79	0.64
1:A:317:MET:HG2	1:A:321:LEU:HD22	1.80	0.64
1:A:464:LEU:HD21	1:A:522:VAL:HG21	1.80	0.63
1:A:565:ASN:C	1:A:567:GLU:H	2.02	0.63
1:A:426:ARG:NH1	2:A:837:HOH:O	2.25	0.63
1:A:136:ASP:OD2	1:A:160:HIS:CD2	2.52	0.63
1:A:560:TYR:HE2	1:A:582:PRO:HD3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TRP:CH2	1:A:232:LEU:HD22	2.34	0.62
1:A:565:ASN:CG	1:A:610:ARG:HG3	2.20	0.62
1:A:351:ILE:O	1:A:355:THR:HB	1.99	0.62
1:A:6:ARG:HD2	1:A:425:VAL:CG2	2.28	0.62
1:A:6:ARG:NH1	1:A:6:ARG:HG3	2.14	0.62
1:A:563:GLU:O	1:A:566:PRO:HG3	1.99	0.62
1:A:527:LEU:HD23	1:A:528:ARG:N	2.15	0.61
1:A:69:LEU:CD1	1:A:101:ALA:HB2	2.27	0.61
1:A:6:ARG:CD	1:A:425:VAL:HG21	2.31	0.61
1:A:407:PHE:HB3	1:A:408:PRO:HD3	1.81	0.61
1:A:267:ARG:O	1:A:271:ARG:HD3	2.00	0.61
1:A:38:ARG:HH11	1:A:457:ASN:HB2	1.65	0.60
1:A:461:LEU:HD23	1:A:508:LEU:HD23	1.83	0.60
1:A:325:ALA:HB3	1:A:334:LEU:HD21	1.82	0.60
1:A:433:LEU:HD21	1:A:636:PHE:HB2	1.84	0.59
1:A:618:VAL:O	1:A:619:LEU:HD23	2.02	0.59
1:A:275:ALA:HA	1:A:306:LEU:HD13	1.84	0.59
1:A:119:MET:HA	1:A:122:VAL:HG23	1.84	0.59
1:A:30:GLU:N	1:A:30:GLU:OE1	2.30	0.58
1:A:373:ALA:HB1	1:A:374:PRO:HD3	1.85	0.58
1:A:491:ALA:HB2	1:A:524:ALA:HB3	1.85	0.58
1:A:560:TYR:CD2	1:A:582:PRO:HD3	2.38	0.58
1:A:613:LEU:N	1:A:613:LEU:HD22	2.19	0.58
1:A:546:LEU:CD2	1:A:606:GLY:HA2	2.32	0.57
1:A:302:GLU:CD	1:A:305:ARG:HH12	2.07	0.57
1:A:34:ALA:HB2	1:A:431:LEU:HD11	1.85	0.57
1:A:139:ILE:HG23	1:A:140:THR:HG23	1.85	0.57
1:A:333:VAL:HB	1:A:411:LYS:HG3	1.87	0.57
1:A:593:PRO:HD2	2:A:843:HOH:O	2.05	0.57
1:A:595:PRO:HB3	1:A:654:TRP:CD1	2.40	0.57
1:A:493:LYS:HG2	1:A:497:LEU:HA	1.87	0.56
1:A:257:TYR:CZ	1:A:259:GLY:HA2	2.39	0.56
1:A:433:LEU:CD2	1:A:632:ARG:HG2	2.28	0.56
1:A:340:HIS:HE1	2:A:759:HOH:O	1.86	0.56
1:A:330:LYS:HE3	2:A:836:HOH:O	2.04	0.56
1:A:493:LYS:HG2	1:A:497:LEU:CA	2.36	0.56
1:A:620:HIS:O	1:A:622:PRO:N	2.40	0.55
1:A:215:ALA:O	1:A:219:ILE:HG12	2.07	0.55
1:A:611:ALA:C	1:A:613:LEU:H	2.10	0.55
1:A:439:LEU:HD21	1:A:620:HIS:CE1	2.41	0.55
1:A:585:ALA:O	1:A:599:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ALA:CB	1:A:424:PRO:HB3	2.36	0.55
1:A:21:VAL:O	1:A:24:ALA:O	2.25	0.55
1:A:565:ASN:C	1:A:567:GLU:N	2.59	0.55
1:A:606:GLY:HA3	1:A:609:ALA:HB2	1.88	0.55
1:A:611:ALA:O	1:A:613:LEU:N	2.40	0.54
1:A:25:LEU:O	1:A:27:VAL:HG13	2.07	0.54
1:A:86:LEU:HD21	1:A:107:ILE:HD12	1.89	0.54
1:A:338:GLU:HB2	2:A:785:HOH:O	2.07	0.54
1:A:478:ARG:HH22	1:A:495:GLY:HA2	1.73	0.54
1:A:583:GLU:C	1:A:599:ARG:HD2	2.27	0.54
1:A:148:LEU:HB2	2:A:825:HOH:O	2.06	0.53
1:A:247:GLY:HA3	1:A:287:LEU:HD22	1.89	0.53
1:A:565:ASN:N	1:A:566:PRO:HD3	2.24	0.53
1:A:457:ASN:ND2	1:A:457:ASN:N	2.38	0.53
1:A:620:HIS:O	1:A:622:PRO:CD	2.56	0.53
1:A:146:ARG:NH1	1:A:149:LEU:HD13	2.23	0.53
1:A:326:ASP:N	1:A:327:PRO:CD	2.65	0.53
1:A:615:ALA:N	1:A:616:PRO:CD	2.72	0.53
1:A:499:LEU:HD22	1:A:499:LEU:N	2.24	0.53
1:A:433:LEU:HB3	1:A:632:ARG:HD3	1.90	0.53
1:A:69:LEU:HD21	1:A:99:LEU:HB2	1.89	0.53
1:A:615:ALA:N	1:A:616:PRO:HD2	2.24	0.53
1:A:612:ARG:O	1:A:612:ARG:HG2	2.09	0.53
1:A:302:GLU:OE1	1:A:305:ARG:NH1	2.42	0.52
1:A:421:PHE:HB3	1:A:422:PRO:HD2	1.91	0.52
1:A:580:LEU:HB2	1:A:585:ALA:HB2	1.91	0.52
1:A:122:VAL:N	1:A:123:PRO:HD2	2.25	0.52
1:A:2:ARG:NH2	1:A:3:ASP:HB3	2.24	0.52
1:A:214:ALA:HB1	1:A:232:LEU:HD21	1.91	0.52
1:A:559:VAL:CG1	1:A:587:LEU:HD23	2.36	0.52
1:A:275:ALA:HB2	1:A:303:LEU:HD22	1.90	0.52
1:A:583:GLU:CA	1:A:599:ARG:HD2	2.40	0.51
1:A:618:VAL:C	1:A:619:LEU:HD23	2.30	0.51
1:A:4:ARG:O	1:A:425:VAL:HG23	2.11	0.51
1:A:459:GLU:HG3	1:A:460:PRO:HD2	1.93	0.51
1:A:329:ALA:C	1:A:331:ALA:H	2.10	0.50
1:A:145:LEU:HB3	1:A:169:PRO:HG2	1.93	0.50
1:A:40:PHE:O	1:A:41:ARG:HG3	2.12	0.50
1:A:620:HIS:O	1:A:622:PRO:HD2	2.11	0.50
1:A:136:ASP:OD2	1:A:160:HIS:HD2	1.92	0.50
1:A:235:GLU:O	1:A:239:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:PRO:C	1:A:624:ALA:N	2.66	0.50
1:A:254:ALA:HB1	1:A:304:HIS:HE1	1.77	0.50
1:A:607:ARG:HG3	1:A:608:GLU:OE1	2.11	0.49
1:A:34:ALA:O	1:A:38:ARG:HG2	2.13	0.49
1:A:440:LEU:HB2	1:A:441:PRO:HD3	1.94	0.49
1:A:477:GLY:O	1:A:479:HIS:N	2.44	0.49
1:A:606:GLY:HA3	1:A:609:ALA:CB	2.42	0.49
1:A:78:HIS:HA	1:A:106:PHE:O	2.12	0.49
1:A:566:PRO:O	1:A:570:ASP:HB2	2.13	0.49
1:A:526:ASP:OD1	1:A:527:LEU:N	2.45	0.49
1:A:607:ARG:HB3	1:A:608:GLU:OE2	2.13	0.49
1:A:629:LEU:HD23	1:A:629:LEU:C	2.32	0.49
1:A:143:ALA:C	1:A:145:LEU:N	2.67	0.48
1:A:134:THR:OG1	1:A:157:VAL:HA	2.13	0.48
1:A:565:ASN:ND2	1:A:567:GLU:CB	2.67	0.48
1:A:565:ASN:CG	1:A:610:ARG:HB2	2.34	0.48
1:A:546:LEU:CD1	1:A:606:GLY:HA2	2.44	0.48
1:A:119:MET:HG2	1:A:144:GLU:OE1	2.14	0.48
1:A:149:LEU:CD2	1:A:150:GLU:N	2.76	0.48
1:A:348:ALA:HB2	1:A:361:LEU:HD22	1.95	0.48
1:A:610:ARG:O	1:A:613:LEU:HB2	2.13	0.48
1:A:594:ARG:CG	1:A:595:PRO:HD2	2.43	0.48
1:A:322:LEU:HB3	1:A:323:PRO:HD3	1.95	0.48
1:A:257:TYR:CE1	1:A:259:GLY:HA2	2.49	0.48
1:A:149:LEU:HD23	1:A:150:GLU:N	2.28	0.47
1:A:145:LEU:CB	1:A:169:PRO:HG2	2.44	0.47
1:A:510:SER:O	1:A:520:TYR:HA	2.13	0.47
1:A:607:ARG:HA	1:A:612:ARG:HD2	1.95	0.47
1:A:307:ASN:OD1	1:A:310:ARG:NH2	2.42	0.47
1:A:42:ARG:HB3	1:A:44:GLU:HG2	1.97	0.47
1:A:326:ASP:H	1:A:327:PRO:CD	2.17	0.47
1:A:150:GLU:O	1:A:151:ASN:CB	2.63	0.47
1:A:2:ARG:HH21	1:A:3:ASP:HB2	1.78	0.47
1:A:425:VAL:HG13	1:A:425:VAL:O	2.14	0.46
1:A:442:GLN:NE2	1:A:442:GLN:HA	2.29	0.46
1:A:38:ARG:HB2	1:A:40:PHE:CD1	2.50	0.46
1:A:555:LEU:HA	1:A:555:LEU:HD12	1.79	0.46
1:A:459:GLU:HG2	1:A:508:LEU:HD22	1.98	0.46
1:A:35:TYR:OH	1:A:449:LEU:HB2	2.16	0.46
1:A:273:ASN:O	1:A:277:ARG:HG2	2.15	0.46
1:A:595:PRO:HA	1:A:654:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:O	1:A:474:LEU:HD23	2.15	0.46
1:A:493:LYS:HG2	1:A:497:LEU:N	2.31	0.46
1:A:546:LEU:CG	1:A:606:GLY:HA2	2.46	0.46
1:A:160:HIS:ND1	1:A:186:THR:HA	2.31	0.46
1:A:376:SER:HB3	1:A:379:GLU:HB2	1.98	0.45
1:A:373:ALA:HB3	1:A:424:PRO:HB3	1.98	0.45
1:A:480:LEU:HD11	1:A:499:LEU:HD21	1.97	0.45
1:A:390:ARG:O	1:A:391:TYR:HB3	2.16	0.45
1:A:464:LEU:HD12	1:A:464:LEU:N	2.31	0.45
1:A:326:ASP:O	1:A:327:PRO:C	2.55	0.45
1:A:496:ASP:O	1:A:497:LEU:O	2.35	0.45
1:A:222:VAL:HG12	1:A:222:VAL:O	2.17	0.45
1:A:126:LEU:HD13	1:A:126:LEU:C	2.37	0.45
1:A:225:LEU:H	1:A:456:GLY:N	2.15	0.45
1:A:497:LEU:O	1:A:498:ALA:O	2.34	0.45
1:A:502:GLU:O	1:A:530:PRO:HD3	2.17	0.45
1:A:340:HIS:CD2	1:A:342:GLY:H	2.21	0.45
1:A:472:ARG:NH1	1:A:488:ARG:HH11	2.15	0.44
1:A:76:ARG:HB2	1:A:104:HIS:CE1	2.52	0.44
1:A:126:LEU:HD22	1:A:153:VAL:HG21	1.99	0.44
1:A:86:LEU:CD2	1:A:107:ILE:HD12	2.47	0.44
1:A:139:ILE:CG1	1:A:163:PRO:HA	2.47	0.44
1:A:465:PHE:CD1	1:A:465:PHE:C	2.90	0.44
1:A:611:ALA:C	1:A:613:LEU:N	2.69	0.44
1:A:30:GLU:CD	1:A:30:GLU:H	2.20	0.44
1:A:142:HIS:CE1	1:A:166:THR:O	2.71	0.44
1:A:607:ARG:CA	1:A:612:ARG:HD2	2.47	0.44
1:A:472:ARG:HH11	1:A:488:ARG:NH1	2.16	0.44
1:A:560:TYR:CE2	1:A:582:PRO:CD	2.92	0.44
1:A:254:ALA:HB1	1:A:304:HIS:CE1	2.51	0.44
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.83	0.44
1:A:565:ASN:OD1	1:A:610:ARG:HB2	2.18	0.43
1:A:149:LEU:CD2	1:A:150:GLU:H	2.31	0.43
1:A:472:ARG:O	1:A:472:ARG:HG3	2.17	0.43
1:A:546:LEU:HB2	1:A:606:GLY:HA2	1.99	0.43
1:A:489:VAL:HA	1:A:522:VAL:O	2.18	0.43
1:A:302:GLU:CD	1:A:305:ARG:NH1	2.70	0.43
1:A:82:ASP:HA	1:A:277:ARG:HH12	1.82	0.43
1:A:653:TYR:HA	1:A:656:VAL:HG22	2.00	0.43
1:A:621:THR:HG23	1:A:622:PRO:CD	2.23	0.43
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:CD1	1:A:626:LEU:HD11	2.48	0.43
1:A:478:ARG:NH2	1:A:495:GLY:HA2	2.32	0.43
1:A:38:ARG:NH1	1:A:457:ASN:HB2	2.30	0.43
1:A:24:ALA:C	1:A:26:GLU:H	2.21	0.43
1:A:494:GLN:HG2	1:A:494:GLN:H	1.38	0.43
1:A:182:LYS:HD3	1:A:182:LYS:HA	1.55	0.43
1:A:543:PRO:HB2	1:A:641:ARG:HA	2.01	0.43
1:A:493:LYS:CG	1:A:497:LEU:H	2.32	0.43
1:A:613:LEU:HA	1:A:613:LEU:HD13	1.57	0.43
1:A:376:SER:HB3	1:A:379:GLU:CB	2.49	0.43
1:A:583:GLU:HA	1:A:599:ARG:CD	2.47	0.43
1:A:557:GLU:O	1:A:559:VAL:HG13	2.19	0.43
1:A:225:LEU:H	1:A:456:GLY:H	1.66	0.42
1:A:613:LEU:N	1:A:613:LEU:CD2	2.80	0.42
1:A:80:ASP:OD2	1:A:81:TYR:N	2.52	0.42
1:A:355:THR:HG23	1:A:357:ARG:HB2	2.00	0.42
1:A:546:LEU:HD13	1:A:606:GLY:CA	2.48	0.42
1:A:119:MET:HA	1:A:122:VAL:CG2	2.49	0.42
1:A:468:PRO:HG3	1:A:499:LEU:HB2	2.01	0.42
1:A:58:LEU:HD11	1:A:194:LEU:HA	2.02	0.42
1:A:497:LEU:O	1:A:498:ALA:HB3	2.20	0.42
1:A:80:ASP:HB3	1:A:85:GLY:HA3	2.01	0.42
1:A:465:PHE:CD2	1:A:504:GLU:HG3	2.54	0.42
1:A:496:ASP:C	1:A:497:LEU:O	2.57	0.42
1:A:180:ASP:O	1:A:181:LEU:C	2.58	0.42
1:A:17:GLN:NE2	1:A:41:ARG:NH2	2.67	0.42
1:A:160:HIS:HA	1:A:174:HIS:CE1	2.55	0.42
1:A:355:THR:CG2	1:A:357:ARG:HB2	2.50	0.42
1:A:352:LEU:C	1:A:352:LEU:HD23	2.41	0.42
1:A:48:PRO:HG2	1:A:231:ALA:HB2	2.01	0.41
1:A:478:ARG:CZ	1:A:495:GLY:HA2	2.50	0.41
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.85	0.41
1:A:442:GLN:HE21	1:A:445:ARG:NH2	2.11	0.41
1:A:352:LEU:O	1:A:356:LEU:N	2.49	0.41
1:A:126:LEU:HD22	1:A:153:VAL:CG2	2.50	0.41
1:A:512:ASN:ND2	1:A:521:GLU:HG3	2.35	0.41
1:A:24:ALA:O	1:A:25:LEU:HB2	2.20	0.41
1:A:585:ALA:C	1:A:599:ARG:HH12	2.23	0.41
1:A:166:THR:O	1:A:166:THR:HG23	2.20	0.41
1:A:174:HIS:HA	1:A:175:PRO:HD3	1.87	0.41
1:A:593:PRO:CD	2:A:843:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLY:CA	1:A:287:LEU:HD22	2.51	0.41
1:A:8:ARG:HD2	2:A:736:HOH:O	2.19	0.41
1:A:493:LYS:HG2	1:A:497:LEU:H	1.86	0.41
1:A:473:ARG:HG2	1:A:474:LEU:N	2.35	0.41
1:A:139:ILE:HG12	1:A:163:PRO:HA	2.03	0.41
1:A:145:LEU:C	1:A:145:LEU:HD12	2.41	0.40
1:A:495:GLY:O	1:A:496:ASP:CB	2.68	0.40
1:A:179:PRO:O	1:A:180:ASP:HB3	2.21	0.40
1:A:358:PRO:HG2	1:A:375:ILE:HD13	2.03	0.40
1:A:53:LEU:HD21	1:A:183:GLU:HG3	2.03	0.40
1:A:159:ASP:OD1	1:A:160:HIS:N	2.52	0.40
1:A:142:HIS:HE1	1:A:166:THR:O	2.04	0.40
1:A:371:SER:OG	1:A:372:LEU:N	2.54	0.40
1:A:620:HIS:HB3	1:A:621:THR:H	1.58	0.40
1:A:76:ARG:HE	1:A:104:HIS:CE1	2.16	0.40
1:A:126:LEU:HD13	1:A:126:LEU:O	2.21	0.40
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.86	0.40
1:A:618:VAL:HB	1:A:619:LEU:H	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	644/666 (97%)	585 (91%)	37 (6%)	22 (3%)	5 6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
1	A	150	GLU
1	A	181	LEU

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Mol	Chain	Res	Type
1	A	325	ALA
1	A	327	PRO
1	A	330	LYS
1	A	373	ALA
1	A	478	ARG
1	A	496	ASP
1	A	620	HIS
1	A	621	THR
1	A	612	ARG
1	A	151	ASN
1	A	152	GLY
1	A	498	ALA
1	A	618	VAL
1	A	623	GLU
1	A	180	ASP
1	A	326	ASP
1	A	609	ALA
1	A	497	LEU
1	A	656	VAL

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	502/516 (97%)	455 (91%)	47 (9%)	11 20

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	ARG
1	A	33	LEU
1	A	44	GLU
1	A	56	LYS
1	A	81	TYR
1	A	127	GLU

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Mol	Chain	Res	Type
1	A	148	LEU
1	A	160	HIS
1	A	171	LEU
1	A	250	LEU
1	A	282	GLU
1	A	283	LYS
1	A	287	LEU
1	A	302	GLU
1	A	321	LEU
1	A	344	MET
1	A	355	THR
1	A	361	LEU
1	A	387	LEU
1	A	430	LEU
1	A	431	LEU
1	A	433	LEU
1	A	457	ASN
1	A	473	ARG
1	A	479	HIS
1	A	487	VAL
1	A	489	VAL
1	A	490	LEU
1	A	494	GLN
1	A	496	ASP
1	A	502	GLU
1	A	509	LEU
1	A	521	GLU
1	A	534	GLU
1	A	555	LEU
1	A	564	ASP
1	A	579	LEU
1	A	599	ARG
1	A	607	ARG
1	A	610	ARG
1	A	621	THR
1	A	623	GLU
1	A	626	LEU
1	A	633	ARG
1	A	640	ARG
1	A	641	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	71	GLN
1	A	78	HIS
1	A	104	HIS
1	A	125	HIS
1	A	141	ASN
1	A	142	HIS
1	A	160	HIS
1	A	161	HIS
1	A	304	HIS
1	A	311	GLN
1	A	340	HIS
1	A	442	GLN
1	A	457	ASN
1	A	565	ASN
1	A	620	HIS

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	648/666 (97%)	0.33	44 (6%)	20	23	13, 37, 76, 90	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.7
1	A	607	ARG	7.2
1	A	621	THR	6.4
1	A	325	ALA	5.5
1	A	608	GLU	5.1
1	A	167	PRO	4.6
1	A	573	TRP	4.6
1	A	152	GLY	4.0
1	A	570	ASP	3.9
1	A	163	PRO	3.8
1	A	162	THR	3.6
1	A	569	LEU	3.4
1	A	126	LEU	3.4
1	A	165	LYS	3.2
1	A	566	PRO	3.2
1	A	572	ALA	3.2
1	A	150	GLU	3.1
1	A	422	PRO	3.1
1	A	574	LYS	3.0
1	A	2	ARG	3.0
1	A	146	ARG	3.0
1	A	599	ARG	3.0
1	A	142	HIS	2.9
1	A	127	GLU	2.8
1	A	25	LEU	2.8
1	A	374	PRO	2.8
1	A	151	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	618	VAL	2.7
1	A	168	PRO	2.7
1	A	166	THR	2.7
1	A	472	ARG	2.7
1	A	326	ASP	2.6
1	A	123	PRO	2.5
1	A	35	TYR	2.5
1	A	107	ILE	2.4
1	A	611	ALA	2.3
1	A	575	ALA	2.2
1	A	474	LEU	2.2
1	A	579	LEU	2.2
1	A	420	ARG	2.2
1	A	140	THR	2.2
1	A	120	GLU	2.1
1	A	182	LYS	2.0
1	A	560	TYR	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.