



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:24 AM UTC

PDB ID : 2ZXO / pdb_00002zxo
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

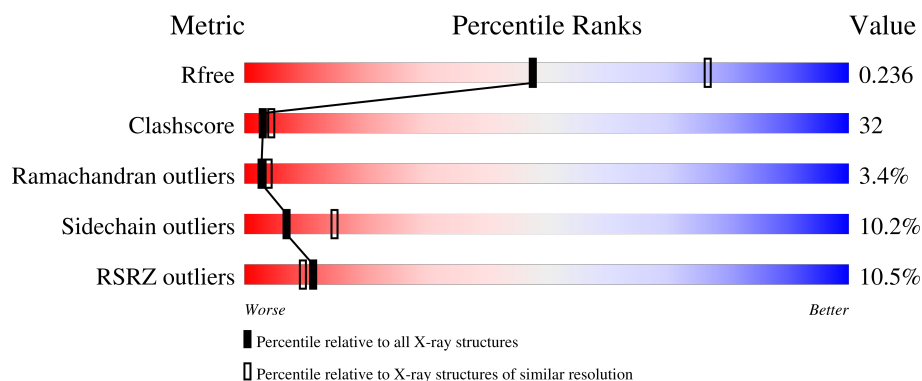
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of 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 $\leq 5\%$. 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	

2 Entry composition

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
1	A	648	Total	C	N	O	S	0	0	0
			5020	3230	903	880	7			

- Molecule 2 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Single-stranded DNA specific exonuclease RecJ



4 Data and refinement statistics

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 42.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.72-2.50) 99.9 (42.72-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	1570 reflections (5.03%)	wwPDB-VP
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 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.71	2/5145 (0.0%)	1.15	38/7012 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	THR	CA-CB	6.97	1.64	1.53
1	A	240	ILE	CA-CB	6.96	1.58	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	SER	N-CA-C	-13.19	96.70	112.92
1	A	24	ALA	N-CA-C	-10.22	97.84	110.41
1	A	624	ALA	N-CA-C	-9.14	100.72	112.23
1	A	329	ALA	N-CA-C	8.46	122.14	112.57
1	A	608	GLU	N-CA-C	-8.01	103.65	113.50
1	A	328	GLU	N-CA-C	-7.48	99.29	109.54
1	A	129	SER	N-CA-C	7.45	120.78	109.23
1	A	321	LEU	N-CA-C	7.28	120.64	111.69
1	A	373	ALA	CA-C-N	-7.24	112.42	120.45
1	A	373	ALA	C-N-CA	-7.24	112.42	120.45
1	A	385	GLU	N-CA-C	6.90	119.64	111.71
1	A	538	ALA	CA-C-N	6.38	126.40	119.90
1	A	538	ALA	C-N-CA	6.38	126.40	119.90
1	A	336	ASP	CA-C-N	6.34	127.77	119.84
1	A	336	ASP	C-N-CA	6.34	127.77	119.84
1	A	380	ALA	N-CA-C	-6.04	104.62	111.14
1	A	559	VAL	N-CA-C	5.98	118.31	108.99
1	A	598	GLY	N-CA-C	-5.95	105.74	114.90
1	A	12	LEU	CA-C-N	-5.93	114.27	120.38
1	A	12	LEU	C-N-CA	-5.93	114.27	120.38
1	A	529	LYS	N-CA-C	-5.90	102.33	109.83
1	A	525	VAL	N-CA-C	-5.81	104.85	113.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	VAL	N-CA-C	5.78	116.62	108.36
1	A	375	ILE	N-CA-C	5.70	116.01	107.51
1	A	591	LEU	N-CA-C	5.68	117.86	109.62
1	A	546	LEU	N-CA-C	5.63	117.10	111.07
1	A	155	VAL	N-CA-C	5.55	115.88	108.11
1	A	507	GLY	N-CA-C	5.53	119.20	110.96
1	A	433	LEU	N-CA-C	-5.53	102.71	110.50
1	A	436	GLU	CA-C-N	5.50	125.85	119.47
1	A	436	GLU	C-N-CA	5.50	125.85	119.47
1	A	491	ALA	N-CA-C	5.45	116.42	108.14
1	A	395	LYS	N-CA-C	5.44	117.97	111.71
1	A	567	GLU	N-CA-C	-5.40	105.48	111.36
1	A	601	VAL	N-CA-C	5.39	116.68	108.80
1	A	616	PRO	CA-C-N	5.37	126.55	119.84
1	A	616	PRO	C-N-CA	5.37	126.55	119.84
1	A	324	GLN	N-CA-C	5.17	117.40	109.95

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	323	0
2	A	180	0	0	17	0
All	All	5200	0	5130	323	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 32.

All (323) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:560:TYR:CE2	1:A:582:PRO:HD3	2.07	0.89
1:A:596:VAL:HG12	1:A:599:ARG:HG3	1.52	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: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:457:ASN:H	1:A:457:ASN:ND2	1.74	0.82
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:60:GLU:CD	1:A:171:LEU:HD21	2.09	0.77
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:566:PRO:HA	1:A:569:LEU:HB3	1.68	0.74
1:A:621:THR:CG2	1:A:622:PRO:HD3	2.16	0.74
1:A:473:ARG:HD3	1:A:475:GLY:O	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:HG3	1:A:6:ARG:HH11	1.52	0.73
1:A:433:LEU:HD23	1:A:632:ARG:CG	2.16	0.73
1:A:565:ASN:ND2	1:A:610:ARG:HG3	2.04	0.73
1:A:2:ARG:HH21	1:A:3:ASP:HB3	1.52	0.72
1:A:442:GLN:NE2	1:A:445:ARG:HH21	1.86	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:46:LEU:O	1:A:230:ARG:NH1	2.23	0.71
1:A:373:ALA:CB	1:A:374:PRO:CD	2.67	0.71
1:A:143:ALA:C	1:A:145:LEU:H	1.99	0.71
1:A:2:ARG:HH21	1:A:3:ASP:CB	2.03	0.71
1:A:622:PRO:C	1:A:624:ALA:H	1.98	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:282:GLU:CD	1:A:282:GLU:H	2.01	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:565:ASN:CG	1:A:610:ARG:HG3	2.20	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:O	1:A:3:ASP:OD2	2.14	0.66
1:A:565:ASN:C	1:A:567:GLU:H	2.02	0.66
1:A:17:GLN:HE21	1:A:36:TRP:HE1	1.42	0.66
1:A:632:ARG:HD2	2:A:812:HOH:O	1.94	0.66
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.26	0.65
1:A:583:GLU:O	1:A:599:ARG:HD2	1.95	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: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: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:228:TRP:CH2	1:A:232:LEU:HD22	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:TYR:HE2	1:A:582:PRO:HD3	1.64	0.62
1:A:351:ILE:O	1:A:355:THR:HB	1.99	0.62
1:A:302:GLU:CD	1:A:305:ARG:HH12	2.07	0.62
1:A:6:ARG:HD2	1:A:425:VAL:CG2	2.28	0.62
1:A:6:ARG:HG3	1:A:6:ARG:NH1	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:6:ARG:CD	1:A:425:VAL:HG21	2.31	0.61
1:A:69:LEU:CD1	1:A:101:ALA:HB2	2.27	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:611:ALA:C	1:A:613:LEU:H	2.10	0.60
1:A:433:LEU:HD21	1:A:636:PHE:HB2	1.84	0.59
1:A:275:ALA:HA	1:A:306:LEU:HD13	1.84	0.59
1:A:565:ASN:C	1:A:567:GLU:N	2.59	0.59
1:A:618:VAL:O	1:A:619:LEU:HD23	2.02	0.59
1:A:119:MET:HA	1:A:122:VAL:HG23	1.84	0.59
1:A:583:GLU:C	1:A:599:ARG:HD2	2.27	0.59
1:A:30:GLU:OE1	1:A:30:GLU:N	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: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:257:TYR:CZ	1:A:259:GLY:HA2	2.39	0.56
1:A:493:LYS:HG2	1:A:497:LEU:HA	1.87	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:618:VAL:C	1:A:619:LEU:HD23	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ALA:C	1:A:331:ALA:H	2.10	0.55
1:A:439:LEU:HD21	1:A:620:HIS:CE1	2.41	0.55
1:A:21:VAL:O	1:A:24:ALA:O	2.25	0.55
1:A:373:ALA:CB	1:A:424:PRO:HB3	2.36	0.55
1:A:585:ALA:O	1:A:599:ARG:NH1	2.40	0.55
1:A:606:GLY:HA3	1:A:609:ALA:HB2	1.88	0.55
1:A:25:LEU:O	1:A:27:VAL:HG13	2.07	0.54
1:A:611:ALA:O	1:A:613:LEU:N	2.40	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: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:457:ASN:N	1:A:457:ASN:ND2	2.38	0.53
1:A:565:ASN:N	1:A:566:PRO:HD3	2.24	0.53
1:A:629:LEU:C	1:A:629:LEU:HD23	2.32	0.53
1:A:143:ALA:C	1:A:145:LEU:N	2.67	0.53
1:A:146:ARG:NH1	1:A:149:LEU:HD13	2.23	0.53
1:A:565:ASN:CG	1:A:610:ARG:HB2	2.34	0.53
1:A:620:HIS:O	1:A:622:PRO:CD	2.56	0.53
1:A:326:ASP:N	1:A:327:PRO:CD	2.65	0.53
1:A:499:LEU:N	1:A:499:LEU:HD22	2.24	0.53
1:A:615:ALA:N	1:A:616:PRO:CD	2.72	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:612:ARG:O	1:A:612:ARG:HG2	2.09	0.53
1:A:615:ALA:N	1:A:616:PRO:HD2	2.24	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:122:VAL:N	1:A:123:PRO:HD2	2.25	0.52
1:A:580:LEU:HB2	1:A:585:ALA:HB2	1.91	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:254:ALA:HB1	1:A:304:HIS:HE1	1.77	0.50
1:A:326:ASP:O	1:A:327:PRO:C	2.55	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:126:LEU:C	1:A:126:LEU:HD13	2.37	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:611:ALA:C	1:A:613:LEU:N	2.69	0.49
1:A:465:PHE:CD1	1:A:465:PHE:C	2.90	0.49
1:A:566:PRO:O	1:A:570:ASP:HB2	2.13	0.49
1:A:30:GLU:H	1:A:30:GLU:CD	2.20	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:134:THR:OG1	1:A:157:VAL:HA	2.13	0.48
1:A:546:LEU:CD1	1:A:606:GLY:HA2	2.44	0.48
1:A:565:ASN:ND2	1:A:567:GLU:CB	2.67	0.48
1:A:119:MET:HG2	1:A:144:GLU:OE1	2.14	0.48
1:A:24:ALA:C	1:A:26:GLU:H	2.21	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:302:GLU:CD	1:A:305:ARG:NH1	2.70	0.48
1:A:322:LEU:HB3	1:A:323:PRO:HD3	1.95	0.48
1:A:594:ARG:CG	1:A:595:PRO:HD2	2.43	0.48
1:A:610:ARG:O	1:A:613:LEU:HB2	2.13	0.48
1:A:622:PRO:C	1:A:624:ALA:N	2.66	0.48
1:A:257:TYR:CE1	1:A:259:GLY:HA2	2.49	0.48
1:A:145:LEU:CB	1:A:169:PRO:HG2	2.44	0.47
1:A:149:LEU:HD23	1:A:150:GLU:N	2.28	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:226:TRP:CD1	2:A:827:HOH:O	2.68	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:613:LEU:C	1:A:615:ALA:H	2.20	0.47
1:A:2:ARG:HH21	1:A:3:ASP:HB2	1.78	0.47
1:A:150:GLU:O	1:A:151:ASN:CB	2.63	0.47
1:A:326:ASP:H	1:A:327:PRO:CD	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASP:C	1:A:497:LEU:O	2.57	0.47
1:A:180:ASP:O	1:A:181:LEU:C	2.58	0.47
1:A:352:LEU:C	1:A:352:LEU:HD23	2.41	0.46
1:A:425:VAL:O	1:A:425:VAL:HG13	2.14	0.46
1:A:442:GLN:NE2	1:A:442:GLN:HA	2.29	0.46
1:A:585:ALA:C	1:A:599:ARG:HH12	2.23	0.46
1:A:38:ARG:HB2	1:A:40:PHE:CD1	2.50	0.46
1:A:555:LEU:HD12	1:A:555:LEU:HA	1.79	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:459:GLU:HG2	1:A:508:LEU:HD22	1.98	0.46
1:A:473:ARG:O	1:A:474:LEU:HD23	2.15	0.46
1:A:595:PRO:HA	1:A:654:TRP:CE2	2.51	0.46
1:A:493:LYS:HG2	1:A:497:LEU:N	2.31	0.46
1:A:160:HIS:ND1	1:A:186:THR:HA	2.31	0.46
1:A:546:LEU:CG	1:A:606:GLY:HA2	2.46	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:145:LEU:C	1:A:145:LEU:HD12	2.41	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:222:VAL:HG12	1:A:222:VAL:O	2.17	0.45
1:A:496:ASP:O	1:A:497:LEU:O	2.35	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:17:GLN:HE21	1:A:36:TRP:NE1	2.13	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: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:432:ASP:CG	1:A:433:LEU:N	2.76	0.44
1:A:472:ARG:HH11	1:A:488:ARG:NH1	2.16	0.44
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.83	0.44
1:A:254:ALA:HB1	1:A:304:HIS:CE1	2.51	0.44
1:A:560:TYR:CE2	1:A:582:PRO:CD	2.92	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:GLU:C	1:A:657:ASN:H	2.26	0.44
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:527:LEU:HD23	1:A:527:LEU:C	2.43	0.43
1:A:565:ASN:OD1	1:A:610:ARG:HB2	2.18	0.43
1:A:82:ASP:HA	1:A:277:ARG:HH12	1.82	0.43
1:A:489:VAL:HA	1:A:522:VAL:O	2.18	0.43
1:A:546:LEU:HB2	1:A:606:GLY:HA2	1.99	0.43
1:A:653:TYR:HA	1:A:656:VAL:HG22	2.00	0.43
1:A:15:LEU:CD1	1:A:626:LEU:HD11	2.48	0.43
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.85	0.43
1:A:621:THR:HG23	1:A:622:PRO:CD	2.23	0.43
1:A:38:ARG:NH1	1:A:457:ASN:HB2	2.30	0.43
1:A:478:ARG:NH2	1:A:495:GLY:HA2	2.32	0.43
1:A:494:GLN:H	1:A:494:GLN:HG2	1.38	0.43
1:A:182:LYS:HA	1:A:182:LYS:HD3	1.55	0.43
1:A:543:PRO:HB2	1:A:641:ARG:HA	2.01	0.43
1:A:40:PHE:C	1:A:41:ARG:HG3	2.44	0.43
1:A:493:LYS:CG	1:A:497:LEU:H	2.32	0.43
1:A:376:SER:HB3	1:A:379:GLU:CB	2.49	0.43
1:A:432:ASP:CG	1:A:433:LEU:H	2.26	0.43
1:A:492:TRP:O	1:A:493:LYS:C	2.62	0.43
1:A:613:LEU:HD13	1:A:613:LEU:HA	1.57	0.43
1:A:557:GLU:O	1:A:559:VAL:HG13	2.19	0.43
1:A:583:GLU:HA	1:A:599:ARG:CD	2.47	0.43
1:A:225:LEU:H	1:A:456:GLY:H	1.66	0.42
1:A:80:ASP:OD2	1:A:81:TYR:N	2.52	0.42
1:A:613:LEU:N	1:A:613:LEU:CD2	2.80	0.42
1:A:355:THR:HG23	1:A:357:ARG:HB2	2.00	0.42
1:A:58:LEU:HD11	1:A:194:LEU:HA	2.02	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:546:LEU:HD13	1:A:606:GLY:CA	2.48	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:497:LEU:O	1:A:498:ALA:HB3	2.20	0.42
1:A:608:GLU:O	1:A:609:ALA:C	2.62	0.42
1:A:540:PHE:CD1	1:A:540:PHE:C	2.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HG2	1:A:231:ALA:HB2	2.01	0.41
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.85	0.41
1:A:478:ARG:CZ	1:A:495:GLY:HA2	2.50	0.41
1:A:352:LEU:O	1:A:356:LEU:N	2.49	0.41
1:A:353:GLU:C	1:A:355:THR:H	2.28	0.41
1:A:442:GLN:HE21	1:A:445:ARG:NH2	2.11	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:175:PRO:C	1:A:177:LEU:H	2.29	0.41
1:A:166:THR:O	1:A:166:THR:HG23	2.20	0.41
1:A:612:ARG:C	1:A:613:LEU:HD22	2.45	0.41
1:A:174:HIS:HA	1:A:175:PRO:HD3	1.87	0.41
1:A:8:ARG:HD2	2:A:736:HOH:O	2.19	0.41
1:A:247:GLY:CA	1:A:287:LEU:HD22	2.51	0.41
1:A:318:LEU:C	1:A:318:LEU:HD13	2.46	0.41
1:A:593:PRO:CD	2:A:843:HOH:O	2.64	0.41
1:A:139:ILE:HG12	1:A:163:PRO:HA	2.03	0.41
1:A:473:ARG:HG2	1:A:474:LEU:N	2.35	0.41
1:A:493:LYS:HG2	1:A:497:LEU:H	1.86	0.41
1:A:495:GLY:O	1:A:496:ASP:CB	2.68	0.40
1:A:53:LEU:HD21	1:A:183:GLU:HG3	2.03	0.40
1:A:179:PRO:O	1:A:180:ASP:HB3	2.21	0.40
1:A:344:MET:HE3	1:A:368:THR:HB	2.03	0.40
1:A:358:PRO:HG2	1:A:375:ILE:HD13	2.03	0.40
1:A:142:HIS:HE1	1:A:166:THR:O	2.04	0.40
1:A:159:ASP:OD1	1:A:160:HIS:N	2.52	0.40
1:A:371:SER:OG	1:A:372:LEU:N	2.54	0.40
1:A:455:GLU:O	1:A:456:GLY:C	2.61	0.40
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.86	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:618:VAL:HB	1:A:619:LEU:H	1.63	0.40
1:A:620:HIS:HB3	1:A:621:THR:H	1.58	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	644/666 (97%)	585 (91%)	37 (6%)	22 (3%)	3 4

All (22) Ramachandran outliers are listed below:

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

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%)	451 (90%)	51 (10%)	7 15

All (51) 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	107	ILE
1	A	127	GLU
1	A	148	LEU
1	A	171	LEU
1	A	172	VAL
1	A	250	LEU
1	A	270	PRO
1	A	282	GLU
1	A	283	LYS
1	A	287	LEU
1	A	302	GLU
1	A	321	LEU
1	A	335	LEU
1	A	344	MET
1	A	353	GLU
1	A	355	THR
1	A	361	LEU
1	A	387	LEU
1	A	414	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	502	GLU
1	A	509	LEU
1	A	521	GLU
1	A	534	GLU
1	A	543	PRO
1	A	555	LEU
1	A	564	ASP
1	A	579	LEU
1	A	597	LEU
1	A	621	THR
1	A	623	GLU
1	A	626	LEU
1	A	629	LEU
1	A	633	ARG
1	A	640	ARG
1	A	641	ARG

Sometimes 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	78	HIS
1	A	104	HIS
1	A	125	HIS
1	A	141	ASN
1	A	142	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	512	ASN
1	A	565	ASN
1	A	620	HIS
1	A	657	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	648/666 (97%)	0.50	68 (10%)	11 10	13, 37, 76, 90	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.3
1	A	621	THR	6.3
1	A	618	VAL	5.3
1	A	325	ALA	5.1
1	A	607	ARG	4.2
1	A	619	LEU	4.1
1	A	326	ASP	4.1
1	A	149	LEU	4.0
1	A	573	TRP	4.0
1	A	609	ALA	3.8
1	A	152	GLY	3.7
1	A	615	ALA	3.7
1	A	123	PRO	3.6
1	A	145	LEU	3.5
1	A	148	LEU	3.4
1	A	608	GLU	3.3
1	A	566	PRO	3.2
1	A	571	TYR	3.2
1	A	147	GLU	3.2
1	A	151	ASN	3.2
1	A	107	ILE	3.1
1	A	599	ARG	3.1
1	A	474	LEU	3.1
1	A	456	GLY	3.1
1	A	25	LEU	3.1
1	A	146	ARG	3.1
1	A	162	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	167	PRO	3.0
1	A	472	ARG	3.0
1	A	327	PRO	2.9
1	A	613	LEU	2.9
1	A	584	GLU	2.9
1	A	150	GLU	2.8
1	A	126	LEU	2.8
1	A	497	LEU	2.8
1	A	139	ILE	2.8
1	A	611	ALA	2.7
1	A	477	GLY	2.6
1	A	2	ARG	2.6
1	A	569	LEU	2.6
1	A	143	ALA	2.6
1	A	654	TRP	2.6
1	A	119	MET	2.5
1	A	606	GLY	2.5
1	A	494	GLN	2.5
1	A	169	PRO	2.4
1	A	561	VAL	2.4
1	A	40	PHE	2.4
1	A	24	ALA	2.4
1	A	165	LYS	2.4
1	A	35	TYR	2.3
1	A	658	ARG	2.3
1	A	166	THR	2.3
1	A	495	GLY	2.3
1	A	144	GLU	2.3
1	A	560	TYR	2.3
1	A	140	THR	2.2
1	A	617	PRO	2.2
1	A	125	HIS	2.2
1	A	622	PRO	2.2
1	A	614	SER	2.2
1	A	108	PRO	2.2
1	A	575	ALA	2.1
1	A	142	HIS	2.1
1	A	579	LEU	2.1
1	A	620	HIS	2.1
1	A	226	TRP	2.1
1	A	574	LYS	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 oligosaccharides 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.