



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 AM GMT

PDB ID : 2ZXR
Title : Crystal structure of RecJ in complex with Mg²⁺ from *Thermus thermophilus* HB8
Authors : Wakamatsu, T.; Kitamura, Y.; Nakagawa, N.; Masui, R.; Kuramitsu, S.
Deposited on : 2009-01-05
Resolution : 2.15 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

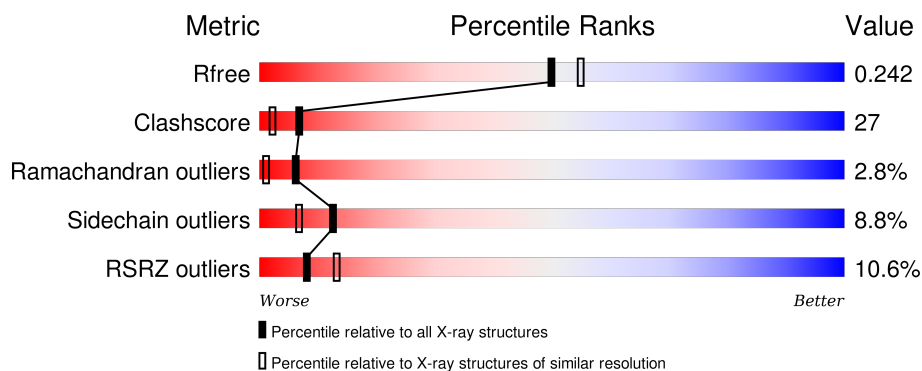
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 $\leq 5\%$. 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	<div> <div>10%</div> <div>60%</div> <div>26%</div> <div>6% • 8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5064 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	616	Total	C	N	O	S	1	0	0
			4773	3077	858	832	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

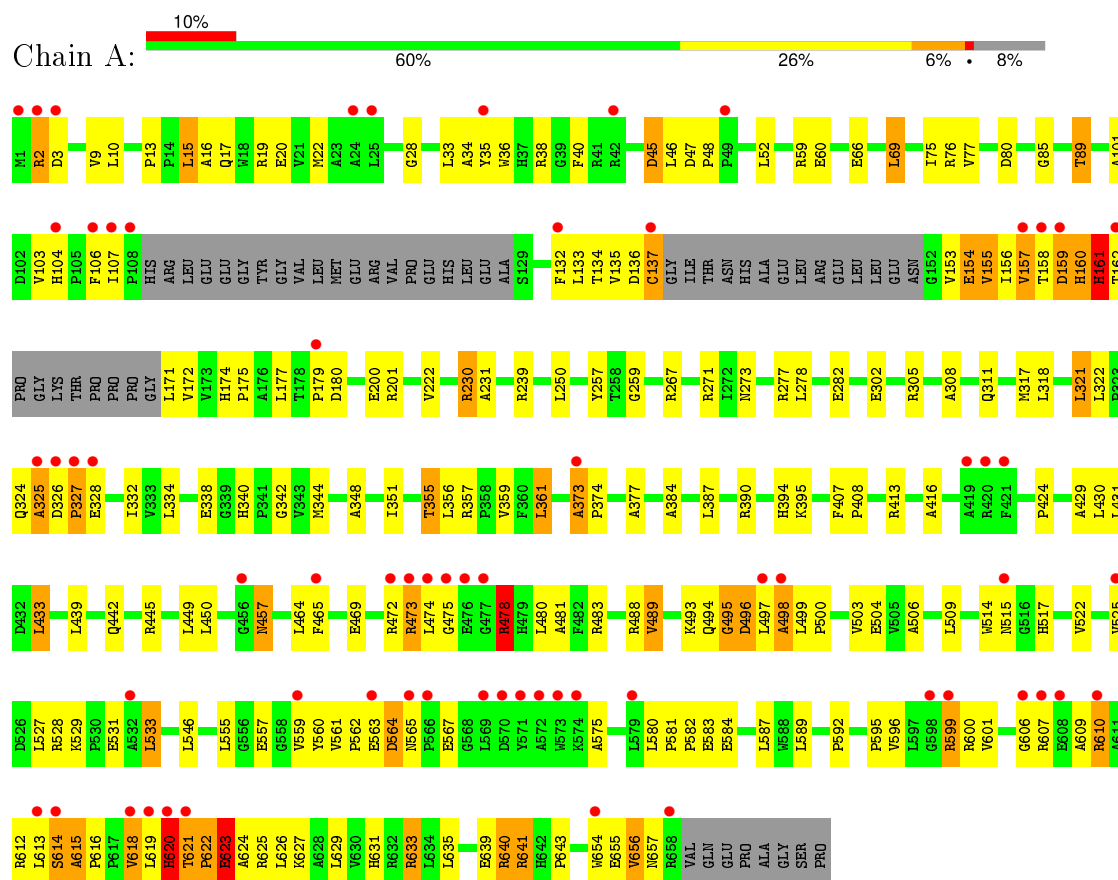
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	290	Total	O	0	0
			290	290		

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 ($\text{RSRZ} > 2$). 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	83.36 Å 83.36 Å 251.06 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 2.15 48.19 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.01-2.15) 98.5 (48.19-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.14 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.279 0.243 , 0.242	Depositor DCC
R_{free} test set	2454 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48586 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5064	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.53	0/4889	0.77	5/6659 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	230	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	230	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	620	HIS	N-CA-C	5.28	125.25	111.00
1	A	239	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	614	SER	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4773	0	4886	260	0
2	A	1	0	0	0	0
3	A	290	0	0	27	0
All	All	5064	0	4886	260	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 27.

All (260) 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:623:GLU:HA	3:A:874:HOH:O	1.44	1.15
1:A:621:THR:HG23	1:A:622:PRO:HD3	1.38	1.01
1:A:457:ASN:HD22	1:A:457:ASN:N	1.57	0.96
1:A:160:HIS:O	1:A:161:HIS:HB2	1.66	0.95
1:A:618:VAL:HG21	3:A:940:HOH:O	1.66	0.94
1:A:546:LEU:HD22	1:A:606:GLY:HA2	1.46	0.94
1:A:373:ALA:HB1	1:A:374:PRO:CD	1.99	0.93
1:A:137:CYS:H	1:A:159:ASP:HB2	1.34	0.92
1:A:135:VAL:HA	1:A:159:ASP:OD1	1.69	0.92
1:A:473:ARG:HH11	1:A:473:ARG:HB2	1.34	0.91
1:A:442:GLN:NE2	1:A:445:ARG:HH21	1.69	0.91
1:A:592:PRO:HG2	1:A:654:TRP:CH2	2.06	0.90
1:A:478:ARG:HH12	1:A:495:GLY:HA2	1.36	0.90
1:A:640:ARG:NH1	1:A:640:ARG:HB2	1.86	0.89
1:A:478:ARG:H	1:A:478:ARG:HD2	1.37	0.89
1:A:457:ASN:HD22	1:A:457:ASN:H	1.19	0.89
1:A:442:GLN:HE21	1:A:445:ARG:HH21	1.18	0.88
1:A:69:LEU:CD2	1:A:101:ALA:HB2	2.05	0.87
1:A:640:ARG:HH11	1:A:640:ARG:HB2	1.40	0.86
1:A:277:ARG:HD3	3:A:907:HOH:O	1.76	0.86
1:A:326:ASP:N	1:A:327:PRO:HD2	1.89	0.85
1:A:137:CYS:O	1:A:157:VAL:HG12	1.77	0.84
1:A:472:ARG:NH1	1:A:488:ARG:HD2	1.93	0.84
1:A:472:ARG:HH11	1:A:488:ARG:HD2	1.42	0.83
1:A:621:THR:HG23	1:A:622:PRO:CD	2.09	0.82
1:A:137:CYS:H	1:A:159:ASP:CB	1.93	0.82
1:A:546:LEU:HD22	1:A:606:GLY:CA	2.09	0.81
1:A:592:PRO:HG2	1:A:654:TRP:HH2	1.46	0.81
1:A:633:ARG:HG2	3:A:837:HOH:O	1.81	0.81
1:A:592:PRO:O	1:A:654:TRP:HZ3	1.65	0.79
1:A:2:ARG:HE	1:A:3:ASP:N	1.79	0.79
1:A:76:ARG:HE	1:A:104:HIS:HE1	1.29	0.79
1:A:340:HIS:HD2	1:A:342:GLY:H	1.32	0.78
1:A:338:GLU:HG3	3:A:863:HOH:O	1.85	0.76
1:A:137:CYS:N	1:A:159:ASP:HB2	2.01	0.76
1:A:517:HIS:HB2	3:A:919:HOH:O	1.85	0.76
1:A:373:ALA:HB2	1:A:424:PRO:HB3	1.67	0.75
1:A:136:ASP:H	1:A:159:ASP:HB3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ALA:CB	1:A:374:PRO:CD	2.65	0.74
1:A:473:ARG:HH11	1:A:473:ARG:CB	2.01	0.73
1:A:326:ASP:OD1	1:A:332:ILE:HD13	1.88	0.73
1:A:478:ARG:NH1	1:A:495:GLY:HA2	2.02	0.73
1:A:328:GLU:HA	3:A:927:HOH:O	1.88	0.72
1:A:457:ASN:ND2	1:A:457:ASN:H	1.85	0.72
1:A:565:ASN:CG	1:A:610:ARG:HB2	2.10	0.72
1:A:134:THR:O	1:A:159:ASP:OD1	2.08	0.71
1:A:134:THR:HG23	3:A:882:HOH:O	1.91	0.71
1:A:85:GLY:O	1:A:89:THR:HG23	1.92	0.70
1:A:609:ALA:O	1:A:613:LEU:HD23	1.89	0.70
1:A:38:ARG:HH11	1:A:457:ASN:HB2	1.55	0.70
1:A:69:LEU:HD21	1:A:101:ALA:HB2	1.74	0.70
1:A:324:GLN:O	1:A:326:ASP:OD2	2.10	0.69
1:A:561:VAL:HG22	1:A:589:LEU:HD12	1.74	0.69
1:A:230:ARG:NH2	1:A:450:LEU:O	2.26	0.69
1:A:132:PHE:HB3	1:A:155:VAL:HG12	1.73	0.69
1:A:373:ALA:HB1	1:A:374:PRO:HD3	1.75	0.69
1:A:609:ALA:HB1	3:A:827:HOH:O	1.92	0.69
1:A:559:VAL:HG12	1:A:587:LEU:HD23	1.75	0.68
1:A:620:HIS:O	1:A:622:PRO:HD2	1.93	0.68
1:A:615:ALA:N	1:A:616:PRO:CD	2.57	0.68
1:A:621:THR:CG2	1:A:622:PRO:HD3	2.21	0.68
1:A:325:ALA:HB3	1:A:334:LEU:HD21	1.74	0.67
1:A:373:ALA:CB	1:A:424:PRO:HB3	2.25	0.67
1:A:332:ILE:HD12	1:A:355:THR:HG21	1.77	0.66
1:A:633:ARG:NH2	3:A:873:HOH:O	2.29	0.66
1:A:15:LEU:HD12	1:A:655:GLU:HB3	1.76	0.65
1:A:17:GLN:NE2	1:A:36:TRP:HE1	1.93	0.65
1:A:442:GLN:HE21	1:A:445:ARG:NH2	1.91	0.65
1:A:583:GLU:HA	1:A:599:ARG:HD2	1.79	0.65
1:A:562:PRO:HG2	3:A:723:HOH:O	1.96	0.65
1:A:473:ARG:HD3	1:A:475:GLY:O	1.98	0.64
1:A:160:HIS:O	1:A:160:HIS:CD2	2.50	0.64
1:A:559:VAL:CG1	1:A:587:LEU:HD23	2.27	0.64
1:A:546:LEU:CD2	1:A:606:GLY:HA2	2.23	0.63
1:A:137:CYS:H	1:A:159:ASP:CG	2.00	0.63
1:A:473:ARG:NH1	1:A:473:ARG:HB2	2.11	0.63
1:A:2:ARG:HE	1:A:3:ASP:CB	2.12	0.63
1:A:546:LEU:HB2	1:A:606:GLY:HA2	1.81	0.63
1:A:2:ARG:NE	1:A:3:ASP:N	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NH1	1:A:457:ASN:HB2	2.14	0.62
1:A:373:ALA:HB1	1:A:374:PRO:HD2	1.82	0.62
1:A:557:GLU:O	1:A:559:VAL:HG13	1.99	0.62
1:A:48:PRO:HG2	1:A:231:ALA:HB2	1.80	0.62
1:A:457:ASN:ND2	1:A:457:ASN:N	2.30	0.62
1:A:473:ARG:HG2	1:A:474:LEU:N	2.14	0.62
1:A:324:GLN:O	1:A:326:ASP:CG	2.38	0.62
1:A:107:ILE:HG21	1:A:282:GLU:HG3	1.80	0.61
1:A:622:PRO:C	1:A:624:ALA:H	2.03	0.61
1:A:15:LEU:HD11	1:A:656:VAL:HG13	1.82	0.61
1:A:80:ASP:OD1	1:A:107:ILE:HD13	2.00	0.61
1:A:133:LEU:CD2	1:A:156:ILE:HB	2.31	0.61
1:A:641:ARG:O	1:A:643:PRO:HD3	2.01	0.60
1:A:478:ARG:HH22	1:A:495:GLY:CA	2.15	0.60
1:A:325:ALA:HB1	3:A:910:HOH:O	2.00	0.60
1:A:136:ASP:H	1:A:159:ASP:CB	2.13	0.60
1:A:472:ARG:HH11	1:A:488:ARG:HH11	1.49	0.59
1:A:9:VAL:HG23	1:A:533:LEU:HD21	1.84	0.59
1:A:277:ARG:HG2	3:A:900:HOH:O	2.03	0.59
1:A:2:ARG:HE	1:A:3:ASP:H	1.48	0.59
1:A:497:LEU:O	1:A:498:ALA:HB3	2.02	0.59
1:A:355:THR:CG2	1:A:357:ARG:HB2	2.33	0.59
1:A:473:ARG:NH2	1:A:497:LEU:HD23	2.19	0.58
1:A:104:HIS:HB3	3:A:880:HOH:O	2.04	0.58
1:A:614:SER:C	1:A:616:PRO:HD2	2.24	0.58
1:A:433:LEU:HD22	1:A:633:ARG:HD3	1.86	0.57
1:A:326:ASP:H	1:A:327:PRO:HD2	1.69	0.57
1:A:344:MET:HE2	1:A:361:LEU:HB3	1.86	0.57
1:A:137:CYS:HA	3:A:946:HOH:O	2.03	0.57
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.35	0.57
1:A:613:LEU:N	1:A:613:LEU:HD22	2.19	0.56
1:A:560:TYR:CE2	1:A:582:PRO:HD3	2.40	0.56
1:A:560:TYR:CD2	1:A:582:PRO:HD3	2.40	0.56
1:A:621:THR:O	1:A:622:PRO:O	2.23	0.56
1:A:157:VAL:HG22	3:A:881:HOH:O	2.05	0.55
1:A:322:LEU:O	1:A:326:ASP:OD2	2.24	0.55
1:A:179:PRO:O	1:A:180:ASP:HB2	2.07	0.55
1:A:384:ALA:HB2	1:A:413:ARG:HG2	1.87	0.55
1:A:38:ARG:HB2	1:A:40:PHE:HD1	1.72	0.55
1:A:592:PRO:O	1:A:654:TRP:CZ3	2.55	0.55
1:A:76:ARG:HE	1:A:104:HIS:CE1	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HG2	3:A:810:HOH:O	2.06	0.55
1:A:497:LEU:HD12	1:A:497:LEU:N	2.22	0.55
1:A:565:ASN:HD21	1:A:567:GLU:HB2	1.72	0.55
1:A:277:ARG:CZ	3:A:906:HOH:O	2.54	0.55
1:A:416:ALA:HA	3:A:951:HOH:O	2.06	0.54
1:A:38:ARG:HB2	1:A:40:PHE:CD1	2.41	0.54
1:A:478:ARG:HH22	1:A:495:GLY:HA2	1.73	0.54
1:A:9:VAL:HG23	1:A:533:LEU:CD2	2.39	0.53
1:A:373:ALA:HB2	3:A:950:HOH:O	2.08	0.53
1:A:514:TRP:CD1	1:A:515:ASN:HB2	2.43	0.53
1:A:16:ALA:O	1:A:20:GLU:HG3	2.09	0.53
1:A:133:LEU:HD22	1:A:156:ILE:HB	1.91	0.53
1:A:172:VAL:HG13	1:A:177:LEU:HD11	1.91	0.53
1:A:160:HIS:C	1:A:160:HIS:CD2	2.81	0.52
1:A:340:HIS:CD2	1:A:342:GLY:H	2.20	0.52
1:A:620:HIS:O	1:A:622:PRO:CD	2.57	0.52
1:A:595:PRO:HD3	1:A:654:TRP:HB3	1.91	0.52
1:A:599:ARG:HE	1:A:599:ARG:HA	1.74	0.52
1:A:618:VAL:O	1:A:619:LEU:HD23	2.10	0.52
1:A:600:ARG:HD2	3:A:830:HOH:O	2.10	0.52
1:A:136:ASP:N	1:A:159:ASP:CB	2.73	0.51
1:A:473:ARG:HG2	1:A:474:LEU:H	1.74	0.51
1:A:529:LYS:O	1:A:531:GLU:HG3	2.10	0.51
1:A:494:GLN:O	1:A:495:GLY:C	2.49	0.51
1:A:2:ARG:NE	1:A:3:ASP:H	2.07	0.51
1:A:311:GLN:NE2	3:A:929:HOH:O	2.39	0.51
1:A:613:LEU:N	1:A:613:LEU:CD2	2.74	0.50
1:A:615:ALA:N	1:A:616:PRO:HD2	2.26	0.50
1:A:439:LEU:HD21	1:A:620:HIS:CE1	2.47	0.50
1:A:527:LEU:HD23	1:A:527:LEU:C	2.32	0.50
1:A:257:TYR:CZ	1:A:259:GLY:HA2	2.46	0.50
1:A:631:HIS:O	1:A:635:LEU:HD23	2.12	0.50
1:A:478:ARG:H	1:A:478:ARG:CD	2.18	0.50
1:A:137:CYS:N	1:A:159:ASP:OD2	2.44	0.50
1:A:34:ALA:O	1:A:38:ARG:HG2	2.12	0.49
1:A:581:PRO:HG2	1:A:584:GLU:HG2	1.93	0.49
1:A:77:VAL:HG12	1:A:89:THR:HB	1.94	0.49
1:A:596:VAL:HG12	1:A:599:ARG:CG	2.42	0.49
1:A:407:PHE:HB3	1:A:408:PRO:HD3	1.95	0.49
1:A:351:ILE:O	1:A:355:THR:HB	2.11	0.49
1:A:494:GLN:HG2	3:A:917:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:MET:HG2	1:A:321:LEU:HD22	1.94	0.49
1:A:222:VAL:HG12	1:A:222:VAL:O	2.12	0.49
1:A:318:LEU:HD22	1:A:322:LEU:HB2	1.95	0.48
1:A:599:ARG:HB3	1:A:601:VAL:HG13	1.95	0.48
1:A:161:HIS:O	1:A:162:THR:CB	2.61	0.48
1:A:267:ARG:O	1:A:271:ARG:HD3	2.14	0.48
1:A:160:HIS:O	1:A:161:HIS:CB	2.47	0.48
1:A:2:ARG:HE	1:A:3:ASP:HB2	1.78	0.48
1:A:277:ARG:NH2	3:A:906:HOH:O	2.46	0.48
1:A:17:GLN:HE21	1:A:36:TRP:HE1	1.61	0.48
1:A:348:ALA:HB2	1:A:361:LEU:HD22	1.96	0.48
1:A:154:GLU:N	1:A:154:GLU:OE2	2.47	0.48
1:A:607:ARG:NE	1:A:607:ARG:HA	2.29	0.48
1:A:158:THR:C	1:A:159:ASP:OD1	2.52	0.48
1:A:308:ALA:HA	1:A:311:GLN:HE21	1.79	0.48
1:A:560:TYR:OH	1:A:592:PRO:HA	2.13	0.47
1:A:478:ARG:NH2	1:A:495:GLY:HA2	2.29	0.47
1:A:13:PRO:HB3	1:A:36:TRP:CD2	2.49	0.47
1:A:76:ARG:CG	1:A:106:PHE:HB2	2.45	0.47
1:A:506:ALA:O	1:A:525:VAL:HG22	2.15	0.47
1:A:174:HIS:ND1	1:A:175:PRO:HD2	2.30	0.47
1:A:478:ARG:NH2	1:A:495:GLY:CA	2.78	0.47
1:A:580:LEU:HD22	1:A:584:GLU:OE1	2.15	0.47
1:A:465:PHE:CD2	1:A:504:GLU:HG3	2.49	0.47
1:A:480:LEU:HD12	1:A:481:ALA:N	2.30	0.47
1:A:332:ILE:CD1	1:A:355:THR:HG21	2.43	0.47
1:A:76:ARG:CD	1:A:106:PHE:HB2	2.45	0.46
1:A:158:THR:O	1:A:159:ASP:OD1	2.34	0.46
1:A:565:ASN:ND2	1:A:567:GLU:HB2	2.30	0.46
1:A:489:VAL:HA	1:A:522:VAL:O	2.15	0.46
1:A:596:VAL:HG12	1:A:599:ARG:HG3	1.96	0.46
1:A:622:PRO:C	1:A:624:ALA:N	2.68	0.46
1:A:483:ARG:HH11	1:A:483:ARG:HG3	1.81	0.46
1:A:40:PHE:CD2	1:A:46:LEU:HD23	2.51	0.46
1:A:302:GLU:OE1	1:A:305:ARG:NH1	2.49	0.46
1:A:592:PRO:CG	1:A:654:TRP:HH2	2.22	0.46
1:A:157:VAL:HG13	3:A:881:HOH:O	2.15	0.45
1:A:326:ASP:O	1:A:327:PRO:O	2.34	0.45
1:A:60:GLU:OE2	1:A:171:LEU:HD22	2.16	0.45
1:A:478:ARG:CZ	1:A:495:GLY:HA2	2.47	0.45
1:A:324:GLN:O	1:A:326:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ARG:HG3	1:A:493:LYS:O	2.15	0.45
1:A:564:ASP:O	1:A:565:ASN:C	2.55	0.45
1:A:500:PRO:HG2	1:A:503:VAL:HG12	1.98	0.45
1:A:546:LEU:CB	1:A:606:GLY:HA2	2.46	0.45
1:A:66:GLU:OE2	1:A:201:ARG:NE	2.45	0.45
1:A:595:PRO:HB3	1:A:654:TRP:CD1	2.52	0.45
1:A:160:HIS:HA	1:A:174:HIS:CD2	2.52	0.45
1:A:499:LEU:HD22	1:A:499:LEU:N	2.31	0.45
1:A:595:PRO:HA	1:A:654:TRP:CE2	2.52	0.44
1:A:172:VAL:O	1:A:172:VAL:HG13	2.17	0.44
1:A:655:GLU:C	1:A:657:ASN:H	2.21	0.44
1:A:28:GLY:HA3	1:A:625:ARG:NH2	2.32	0.44
1:A:19:ARG:HA	1:A:22:MET:HE3	1.98	0.44
1:A:158:THR:C	1:A:159:ASP:CG	2.75	0.44
1:A:359:VAL:HG12	1:A:361:LEU:HD13	2.00	0.44
1:A:15:LEU:CD1	1:A:655:GLU:HB3	2.46	0.44
1:A:480:LEU:HD12	1:A:480:LEU:C	2.38	0.44
1:A:282:GLU:H	1:A:282:GLU:CD	2.20	0.44
1:A:495:GLY:O	1:A:496:ASP:CB	2.66	0.43
1:A:326:ASP:N	1:A:327:PRO:CD	2.72	0.43
1:A:355:THR:HG23	1:A:357:ARG:HB2	2.01	0.43
1:A:384:ALA:CB	1:A:413:ARG:HG2	2.48	0.43
1:A:13:PRO:HB3	1:A:36:TRP:CE3	2.53	0.43
1:A:635:LEU:O	1:A:639:GLU:HG3	2.19	0.43
1:A:610:ARG:O	1:A:613:LEU:HB2	2.19	0.43
1:A:35:TYR:OH	1:A:449:LEU:HB2	2.19	0.43
1:A:273:ASN:O	1:A:277:ARG:HG3	2.19	0.43
1:A:45:ASP:OD1	1:A:45:ASP:N	2.52	0.43
1:A:177:LEU:O	1:A:179:PRO:HD3	2.19	0.43
1:A:327:PRO:HB2	1:A:328:GLU:H	1.57	0.42
1:A:449:LEU:N	1:A:449:LEU:HD22	2.34	0.42
1:A:136:ASP:O	1:A:137:CYS:HB2	2.18	0.42
1:A:613:LEU:C	1:A:616:PRO:HD3	2.39	0.42
1:A:496:ASP:C	1:A:497:LEU:O	2.56	0.42
1:A:75:ILE:O	1:A:103:VAL:HA	2.18	0.42
1:A:527:LEU:HD23	1:A:528:ARG:N	2.35	0.42
1:A:563:GLU:HA	1:A:563:GLU:OE2	2.20	0.42
1:A:136:ASP:N	1:A:159:ASP:CG	2.74	0.41
1:A:559:VAL:HG11	1:A:587:LEU:HD23	2.03	0.41
1:A:136:ASP:N	1:A:159:ASP:HB3	2.27	0.41
1:A:10:LEU:HD21	1:A:429:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD22	1:A:200:GLU:HG3	2.03	0.41
1:A:136:ASP:OD2	1:A:160:HIS:O	2.38	0.41
1:A:161:HIS:O	1:A:162:THR:HB	2.20	0.41
1:A:640:ARG:HB2	1:A:640:ARG:CZ	2.48	0.41
1:A:133:LEU:HD21	1:A:156:ILE:HD12	2.03	0.41
1:A:180:ASP:N	3:A:885:HOH:O	2.53	0.41
1:A:464:LEU:HD12	1:A:464:LEU:N	2.36	0.41
1:A:612:ARG:C	1:A:614:SER:H	2.24	0.41
1:A:473:ARG:NH2	1:A:497:LEU:CD2	2.84	0.41
1:A:59:ARG:NH1	3:A:784:HOH:O	2.53	0.41
1:A:433:LEU:CD2	1:A:633:ARG:HD3	2.48	0.41
1:A:326:ASP:O	1:A:327:PRO:C	2.58	0.40
1:A:629:LEU:C	1:A:629:LEU:HD23	2.40	0.40
1:A:355:THR:HG23	1:A:357:ARG:CG	2.51	0.40
1:A:76:ARG:CD	1:A:132:PHE:HE1	2.34	0.40
1:A:478:ARG:N	1:A:478:ARG:HD2	2.17	0.40
1:A:377:ALA:HB3	1:A:394:HIS:O	2.20	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	608/666 (91%)	563 (93%)	28 (5%)	17 (3%)	6 1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	325	ALA
1	A	327	PRO
1	A	373	ALA

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Mol	Chain	Res	Type
1	A	496	ASP
1	A	620	HIS
1	A	621	THR
1	A	478	ARG
1	A	495	GLY
1	A	618	VAL
1	A	622	PRO
1	A	575	ALA
1	A	623	GLU
1	A	153	VAL
1	A	498	ALA
1	A	656	VAL
1	A	615	ALA

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	475/516 (92%)	433 (91%)	42 (9%)	12 7

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	15	LEU
1	A	33	LEU
1	A	45	ASP
1	A	47	ASP
1	A	69	LEU
1	A	89	THR
1	A	137	CYS
1	A	154	GLU
1	A	155	VAL
1	A	157	VAL
1	A	159	ASP
1	A	160	HIS

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Mol	Chain	Res	Type
1	A	161	HIS
1	A	250	LEU
1	A	278	LEU
1	A	321	LEU
1	A	355	THR
1	A	356	LEU
1	A	361	LEU
1	A	387	LEU
1	A	390	ARG
1	A	430	LEU
1	A	431	LEU
1	A	433	LEU
1	A	457	ASN
1	A	469	GLU
1	A	473	ARG
1	A	478	ARG
1	A	489	VAL
1	A	509	LEU
1	A	533	LEU
1	A	555	LEU
1	A	564	ASP
1	A	599	ARG
1	A	610	ARG
1	A	623	GLU
1	A	626	LEU
1	A	627	LYS
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	71	GLN
1	A	104	HIS
1	A	160	HIS
1	A	304	HIS
1	A	311	GLN
1	A	340	HIS
1	A	394	HIS
1	A	442	GLN

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Mol	Chain	Res	Type
1	A	457	ASN
1	A	517	HIS
1	A	565	ASN
1	A	620	HIS
1	A	631	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	616/666 (92%)	0.83	65 (10%) 8 13	15, 31, 58, 72	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	607	ARG	10.5
1	A	1	MET	9.1
1	A	621	THR	8.1
1	A	159	ASP	6.9
1	A	608	GLU	5.8
1	A	158	THR	5.8
1	A	2	ARG	5.5
1	A	325	ALA	5.4
1	A	565	ASN	5.1
1	A	572	ALA	5.0
1	A	108	PRO	5.0
1	A	573	TRP	4.9
1	A	107	ILE	4.9
1	A	475	GLY	4.7
1	A	157	VAL	4.7
1	A	570	ASP	4.4
1	A	613	LEU	4.2
1	A	599	ARG	4.0
1	A	606	GLY	3.9
1	A	162	THR	3.9
1	A	569	LEU	3.7
1	A	179	PRO	3.6
1	A	532	ALA	3.6
1	A	477	GLY	3.5
1	A	566	PRO	3.5
1	A	574	LYS	3.5
1	A	327	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	610	ARG	3.3
1	A	419	ALA	3.3
1	A	619	LEU	3.2
1	A	473	ARG	3.1
1	A	456	GLY	3.1
1	A	476	GLU	3.0
1	A	106	PHE	3.0
1	A	25	LEU	3.0
1	A	24	ALA	3.0
1	A	515	ASN	3.0
1	A	472	ARG	2.8
1	A	618	VAL	2.8
1	A	563	GLU	2.8
1	A	474	LEU	2.7
1	A	497	LEU	2.7
1	A	35	TYR	2.7
1	A	373	ALA	2.7
1	A	42	ARG	2.7
1	A	465	PHE	2.7
1	A	620	HIS	2.7
1	A	328	GLU	2.6
1	A	326	ASP	2.6
1	A	104	HIS	2.6
1	A	498	ALA	2.5
1	A	579	LEU	2.5
1	A	654	TRP	2.4
1	A	571	TYR	2.4
1	A	559	VAL	2.3
1	A	525	VAL	2.3
1	A	420	ARG	2.3
1	A	137	CYS	2.3
1	A	658	ARG	2.3
1	A	598	GLY	2.1
1	A	132	PHE	2.1
1	A	421	PHE	2.1
1	A	3	ASP	2.1
1	A	614	SER	2.0
1	A	49	PRO	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	667	1/1	0.99	0.15	-0.33	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.