



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:06 PM UTC

PDB ID : 2ZXR / pdb_00002zxr
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

<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

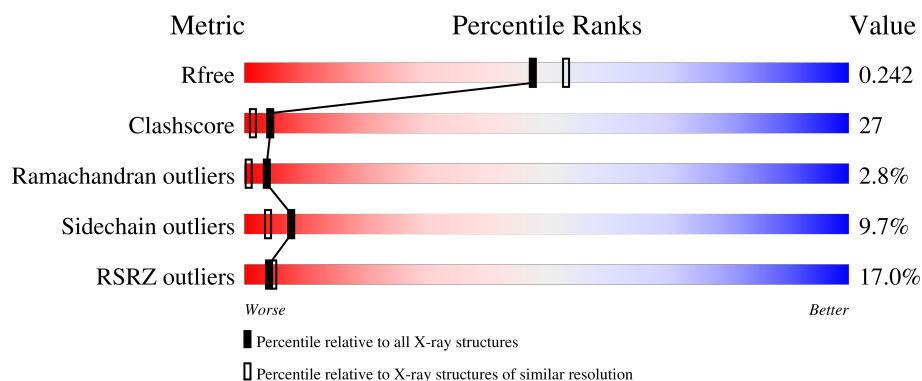
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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	16% 58% 27% 6% • 8%

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 (CCD ID: MG) (formula: Mg).

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

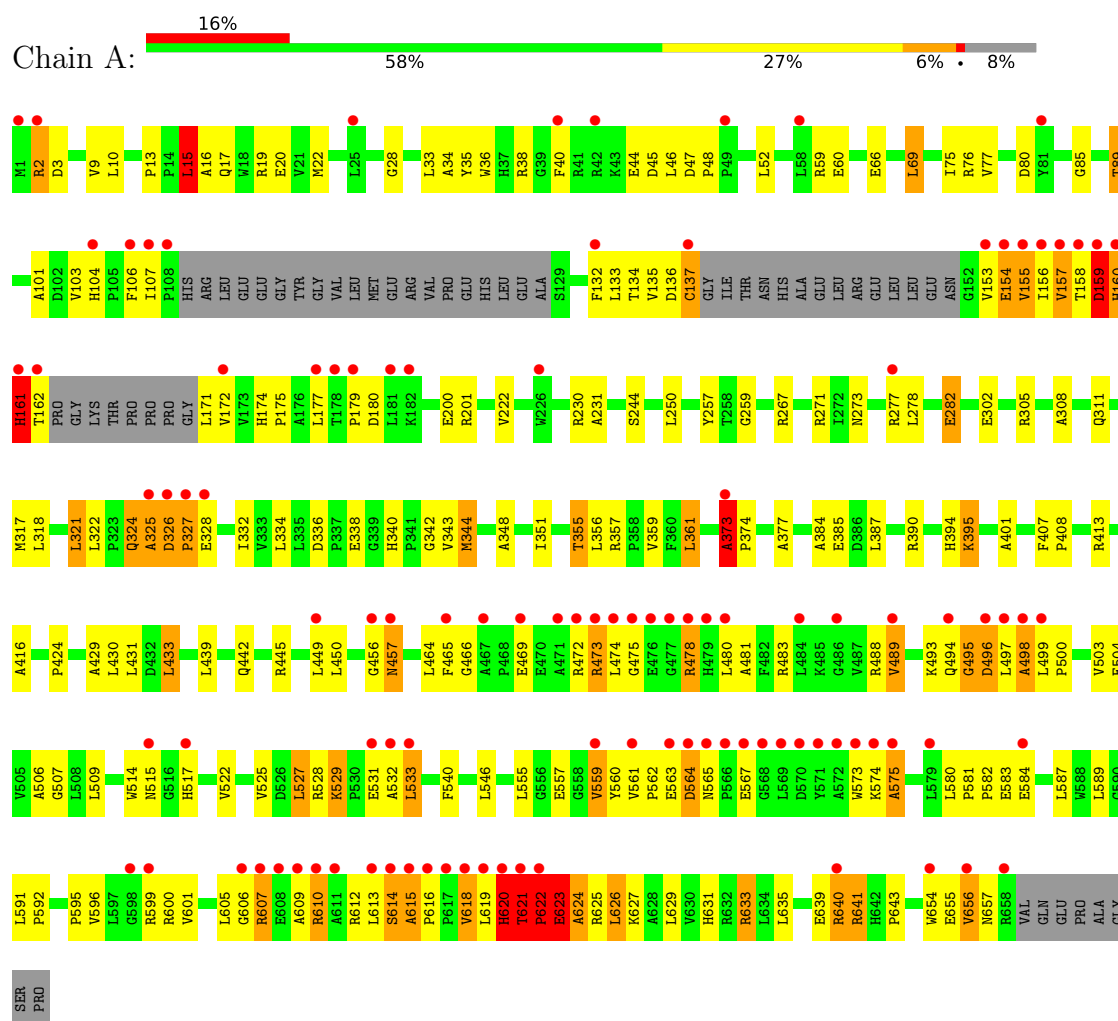
- Molecule 3 is water.

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

3 Residue-property plots [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	83.36Å 83.36Å 251.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 2.15 43.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.01-2.15) 98.5 (43.01-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.279 0.243 , 0.242	Depositor DCC
R_{free} test set	2459 reflections (4.98%)	wwPDB-VP
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 , 42.7	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	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.65	1/4889 (0.0%)	1.11	28/6659 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	THR	CA-CB	5.25	1.61	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	SER	N-CA-C	-10.97	97.48	112.94
1	A	159	ASP	N-CA-C	10.10	121.57	108.24
1	A	607	ARG	N-CA-C	-9.18	104.16	114.62
1	A	373	ALA	CA-C-N	-8.93	110.76	120.94
1	A	373	ALA	C-N-CA	-8.93	110.76	120.94
1	A	529	LYS	N-CA-C	-8.57	98.95	109.83
1	A	385	GLU	N-CA-C	7.56	120.41	111.71
1	A	324	GLN	N-CA-C	7.24	121.08	110.59
1	A	620	HIS	N-CA-C	6.78	125.25	110.80
1	A	621	THR	CA-C-N	-6.73	111.43	119.84
1	A	621	THR	C-N-CA	-6.73	111.43	119.84
1	A	624	ALA	N-CA-C	-6.56	104.21	111.82
1	A	507	GLY	N-CA-C	6.26	120.29	110.96
1	A	15	LEU	N-CA-C	5.86	118.14	111.11
1	A	540	PHE	N-CA-C	-5.74	107.52	114.75
1	A	395	LYS	N-CA-C	5.65	118.21	111.71
1	A	244	SER	N-CA-C	-5.65	106.35	113.18
1	A	626	LEU	N-CA-C	-5.64	105.22	111.36
1	A	326	ASP	N-CA-C	5.53	122.03	109.81
1	A	559	VAL	N-CA-C	5.52	117.75	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	LEU	N-CA-C	-5.42	104.86	112.12
1	A	336	ASP	CA-C-N	5.32	126.48	119.84
1	A	336	ASP	C-N-CA	5.32	126.48	119.84
1	A	456	GLY	N-CA-C	5.31	118.91	112.49
1	A	401	ALA	N-CA-C	-5.24	101.22	109.50
1	A	466	GLY	N-CA-C	5.20	117.77	110.38
1	A	591	LEU	CA-C-N	-5.10	115.13	120.38
1	A	591	LEU	C-N-CA	-5.10	115.13	120.38

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	4773	0	4886	262	0
2	A	1	0	0	0	0
3	A	290	0	0	27	0
All	All	5064	0	4886	262	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 (262) 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:N	1:A:457:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:640:ARG:NH1	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:HB2	1:A:640:ARG:HH11	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:565:ASN:CG	1:A:610:ARG:HB2	2.10	0.76
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
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:H	1:A:457:ASN:ND2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HD21	1:A:101:ALA:HB2	1.74	0.70
1:A:137:CYS:H	1:A:159:ASP:CG	2.00	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:615:ALA:N	1:A:616:PRO:CD	2.57	0.68
1:A:620:HIS:O	1:A:622:PRO:HD2	1.93	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:622:PRO:C	1:A:624:ALA:H	2.03	0.67
1:A:324:GLN:O	1:A:326:ASP:CG	2.38	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:2:ARG:HE	1:A:3:ASP:CB	2.12	0.63
1:A:473:ARG:HB2	1:A:473:ARG:NH1	2.11	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
1:A:38:ARG:NH1	1:A:457:ASN:HB2	2.14	0.62
1:A:614:SER:C	1:A:616:PRO:HD2	2.24	0.62
1:A:373:ALA:HB1	1:A:374:PRO:HD2	1.82	0.62
1:A:48:PRO:HG2	1:A:231:ALA:HB2	1.80	0.62
1:A:557:GLU:O	1:A:559:VAL:HG13	1.99	0.62
1:A:473:ARG:HG2	1:A:474:LEU:N	2.14	0.62
1:A:107:ILE:HG21	1:A:282:GLU:HG3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:ARG:HE	1:A:3:ASP:H	1.48	0.59
1:A:277:ARG:HG2	3:A:900:HOH:O	2.03	0.59
1:A:355:THR:CG2	1:A:357:ARG:HB2	2.33	0.59
1:A:497:LEU:O	1:A:498:ALA:HB3	2.02	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:433:LEU:HD22	1:A:633:ARG:HD3	1.86	0.57
1:A:160:HIS:CD2	1:A:160:HIS:C	2.81	0.57
1:A:326:ASP:H	1:A:327:PRO:HD2	1.69	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:344:MET:HE2	1:A:361:LEU:HB3	1.87	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:494:GLN:O	1:A:495:GLY:C	2.49	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:76:ARG:HE	1:A:104:HIS:CE1	2.18	0.55
1:A:395:LYS:HG2	3:A:810:HOH:O	2.06	0.55
1:A:592:PRO:O	1:A:654:TRP:CZ3	2.55	0.55
1:A:497:LEU:N	1:A:497:LEU:HD12	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:527:LEU:C	1:A:527:LEU:HD23	2.32	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:158:THR:C	1:A:159:ASP:CG	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:O	1:A:20:GLU:HG3	2.09	0.53
1:A:179:PRO:O	1:A:180:ASP:HB2	2.07	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:158:THR:C	1:A:159:ASP:OD1	2.52	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:600:ARG:HD2	3:A:830:HOH:O	2.10	0.52
1:A:618:VAL:O	1:A:619:LEU:HD23	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: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: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:564:ASP:O	1:A:565:ASN:C	2.55	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:407:PHE:HB3	1:A:408:PRO:HD3	1.95	0.49
1:A:596:VAL:HG12	1:A:599:ARG:CG	2.42	0.49
1:A:351:ILE:O	1:A:355:THR:HB	2.11	0.49
1:A:655:GLU:C	1:A:657:ASN:H	2.21	0.49
1:A:494:GLN:HG2	3:A:917:HOH:O	2.12	0.49
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:282:GLU:CD	1:A:282:GLU:H	2.20	0.48
1:A:2:ARG:HE	1:A:3:ASP:HB2	1.78	0.48
1:A:160:HIS:O	1:A:161:HIS:CB	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:C	1:A:480:LEU:HD12	2.38	0.48
1:A:17:GLN:HE21	1:A:36:TRP:HE1	1.61	0.48
1:A:277:ARG:NH2	3:A:906:HOH:O	2.46	0.48
1:A:154:GLU:N	1:A:154:GLU:OE2	2.47	0.48
1:A:348:ALA:HB2	1:A:361:LEU:HD22	1.96	0.48
1:A:607:ARG:HA	1:A:607:ARG:NE	2.29	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:13:PRO:HB3	1:A:36:TRP:CD2	2.49	0.47
1:A:478:ARG:NH2	1:A:495:GLY:HA2	2.29	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:465:PHE:CD2	1:A:504:GLU:HG3	2.49	0.47
1:A:478:ARG:NH2	1:A:495:GLY:CA	2.78	0.47
1:A:480:LEU:HD12	1:A:481:ALA:N	2.30	0.47
1:A:496:ASP:C	1:A:497:LEU:O	2.56	0.47
1:A:580:LEU:HD22	1:A:584:GLU:OE1	2.15	0.47
1:A:613:LEU:C	1:A:616:PRO:HD3	2.39	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:136:ASP:N	1:A:159:ASP:CG	2.74	0.46
1:A:158:THR:O	1:A:159:ASP:OD1	2.34	0.46
1:A:489:VAL:HA	1:A:522:VAL:O	2.15	0.46
1:A:565:ASN:ND2	1:A:567:GLU:HB2	2.30	0.46
1:A:596:VAL:HG12	1:A:599:ARG:HG3	1.96	0.46
1:A:483:ARG:HG3	1:A:483:ARG:HH11	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:612:ARG:C	1:A:614:SER:H	2.24	0.46
1:A:60:GLU:OE2	1:A:171:LEU:HD22	2.16	0.45
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:629:LEU:C	1:A:629:LEU:HD23	2.40	0.45
1:A:324:GLN:O	1:A:326:ASP:N	2.49	0.45
1:A:478:ARG:CZ	1:A:495:GLY:HA2	2.47	0.45
1:A:326:ASP:O	1:A:327:PRO:C	2.58	0.45
1:A:478:ARG:HG3	1:A:493:LYS:O	2.15	0.45
1:A:500:PRO:HG2	1:A:503:VAL:HG12	1.98	0.45
1:A:622:PRO:C	1:A:624:ALA:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE2	1:A:201:ARG:NE	2.45	0.45
1:A:546:LEU:CB	1:A:606:GLY:HA2	2.46	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:N	1:A:499:LEU:HD22	2.31	0.45
1:A:172:VAL:HG13	1:A:172:VAL:O	2.17	0.44
1:A:595:PRO:HA	1:A:654:TRP:CE2	2.52	0.44
1:A:28:GLY:HA3	1:A:625:ARG:NH2	2.32	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: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:45:ASP:OD1	1:A:45:ASP:N	2.52	0.43
1:A:273:ASN:O	1:A:277:ARG:HG3	2.19	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:HD22	1:A:449:LEU:N	2.34	0.42
1:A:136:ASP:O	1:A:137:CYS:HB2	2.18	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:OE2	1:A:563:GLU:HA	2.20	0.42
1:A:495:GLY:O	1:A:496:ASP:CG	2.63	0.41
1:A:531:GLU:O	1:A:532:ALA:C	2.63	0.41
1:A:559:VAL:HG11	1:A:587:LEU:HD23	2.03	0.41
1:A:10:LEU:HD21	1:A:429:ALA:HB1	2.01	0.41
1:A:136:ASP:N	1:A:159:ASP:HB3	2.27	0.41
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:133:LEU:HD21	1:A:156:ILE:HD12	2.03	0.41
1:A:161:HIS:O	1:A:162:THR:HB	2.20	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:640:ARG:HB2	1:A:640:ARG:CZ	2.48	0.41
1:A:59:ARG:NH1	3:A:784:HOH:O	2.53	0.41
1:A:473:ARG:NH2	1:A:497:LEU:CD2	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:CD2	1:A:633:ARG:HD3	2.48	0.41
1:A:19:ARG:HA	1:A:22:MET:HE3	2.03	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:377:ALA:HB3	1:A:394:HIS:O	2.20	0.40
1:A:478:ARG:HD2	1:A:478:ARG:N	2.17	0.40
1:A:573:TRP:C	1:A:575:ALA:H	2.30	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	608/666 (91%)	563 (93%)	28 (5%)	17 (3%)	4 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
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

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Mol	Chain	Res	Type
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%)	429 (90%)	46 (10%)	8 4

All (46) 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	44	GLU
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
1	A	161	HIS
1	A	250	LEU
1	A	278	LEU
1	A	282	GLU
1	A	321	LEU
1	A	343	VAL
1	A	344	MET
1	A	355	THR
1	A	356	LEU
1	A	361	LEU

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Mol	Chain	Res	Type
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	489	VAL
1	A	509	LEU
1	A	527	LEU
1	A	533	LEU
1	A	555	LEU
1	A	564	ASP
1	A	574	LYS
1	A	610	ARG
1	A	622	PRO
1	A	623	GLU
1	A	626	LEU
1	A	627	LYS
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 (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
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 oligosaccharides 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%)	0.85	105 (17%) 4 5	15, 31, 58, 72	1 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.6
1	A	159	ASP	8.5
1	A	619	LEU	8.4
1	A	621	THR	8.1
1	A	158	THR	7.6
1	A	607	ARG	6.8
1	A	157	VAL	6.8
1	A	162	THR	6.2
1	A	609	ALA	5.9
1	A	613	LEU	5.9
1	A	107	ILE	5.8
1	A	497	LEU	5.3
1	A	606	GLY	5.3
1	A	2	ARG	5.2
1	A	327	PRO	5.1
1	A	608	GLU	5.1
1	A	325	ALA	5.0
1	A	618	VAL	5.0
1	A	565	ASN	5.0
1	A	475	GLY	4.9
1	A	573	TRP	4.8
1	A	599	ARG	4.8
1	A	474	LEU	4.8
1	A	610	ARG	4.6
1	A	456	GLY	4.3
1	A	477	GLY	4.3
1	A	108	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	471	ALA	4.2
1	A	498	ALA	4.2
1	A	106	PHE	4.1
1	A	532	ALA	4.1
1	A	620	HIS	4.0
1	A	615	ALA	3.9
1	A	154	GLU	3.9
1	A	617	PRO	3.8
1	A	326	ASP	3.8
1	A	465	PHE	3.8
1	A	473	ARG	3.8
1	A	137	CYS	3.8
1	A	373	ALA	3.7
1	A	622	PRO	3.6
1	A	564	ASP	3.5
1	A	153	VAL	3.5
1	A	598	GLY	3.5
1	A	161	HIS	3.5
1	A	476	GLU	3.5
1	A	156	ILE	3.4
1	A	104	HIS	3.4
1	A	277	ARG	3.4
1	A	160	HIS	3.3
1	A	614	SER	3.3
1	A	654	TRP	3.3
1	A	472	ARG	3.3
1	A	178	THR	3.2
1	A	515	ASN	3.2
1	A	656	VAL	3.2
1	A	81	TYR	3.1
1	A	570	ASP	3.1
1	A	496	ASP	3.1
1	A	328	GLU	3.0
1	A	611	ALA	3.0
1	A	179	PRO	3.0
1	A	155	VAL	2.9
1	A	172	VAL	2.9
1	A	494	GLN	2.9
1	A	575	ALA	2.8
1	A	42	ARG	2.7
1	A	480	LEU	2.7
1	A	533	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	PHE	2.7
1	A	467	ALA	2.7
1	A	579	LEU	2.7
1	A	563	GLU	2.7
1	A	658	ARG	2.6
1	A	517	HIS	2.5
1	A	574	LYS	2.5
1	A	572	ALA	2.5
1	A	226	TRP	2.5
1	A	181	LEU	2.4
1	A	571	TYR	2.4
1	A	566	PRO	2.4
1	A	177	LEU	2.4
1	A	569	LEU	2.4
1	A	584	GLU	2.4
1	A	40	PHE	2.4
1	A	49	PRO	2.4
1	A	25	LEU	2.3
1	A	478	ARG	2.3
1	A	58	LEU	2.2
1	A	469	GLU	2.2
1	A	182	LYS	2.2
1	A	499	LEU	2.2
1	A	489	VAL	2.1
1	A	479	HIS	2.1
1	A	561	VAL	2.1
1	A	449	LEU	2.1
1	A	531	GLU	2.0
1	A	457	ASN	2.0
1	A	640	ARG	2.0
1	A	616	PRO	2.0
1	A	568	GLY	2.0
1	A	559	VAL	2.0
1	A	567	GLU	2.0
1	A	484	LEU	2.0
1	A	486	GLY	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	667	1/1	0.99	0.05	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.