



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:04 PM UTC

PDB ID : 2ZXP / pdb_00002zxp
Title : Crystal structure of RecJ in complex with Mn²⁺ from *Thermus thermophilus* HB8
Authors : Wakamatsu, T.; Kitamura, Y.; Nakagawa, N.; Masui, R.; Kuramitsu, S.
Deposited on : 2009-01-05
Resolution : 2.30 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

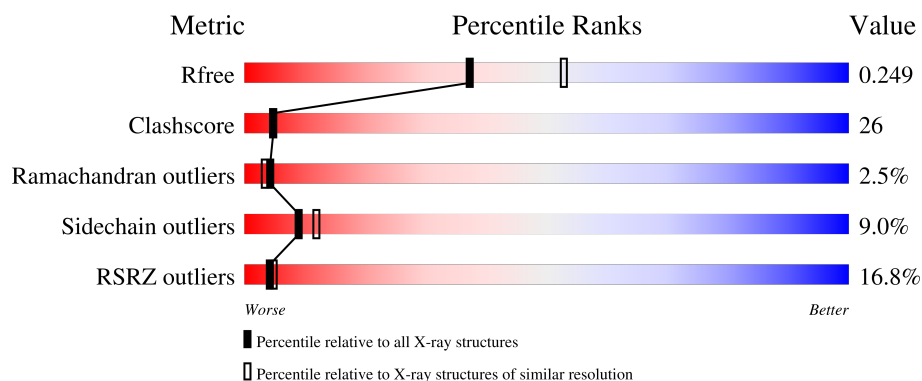
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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% 60% 30% 6% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5315 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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

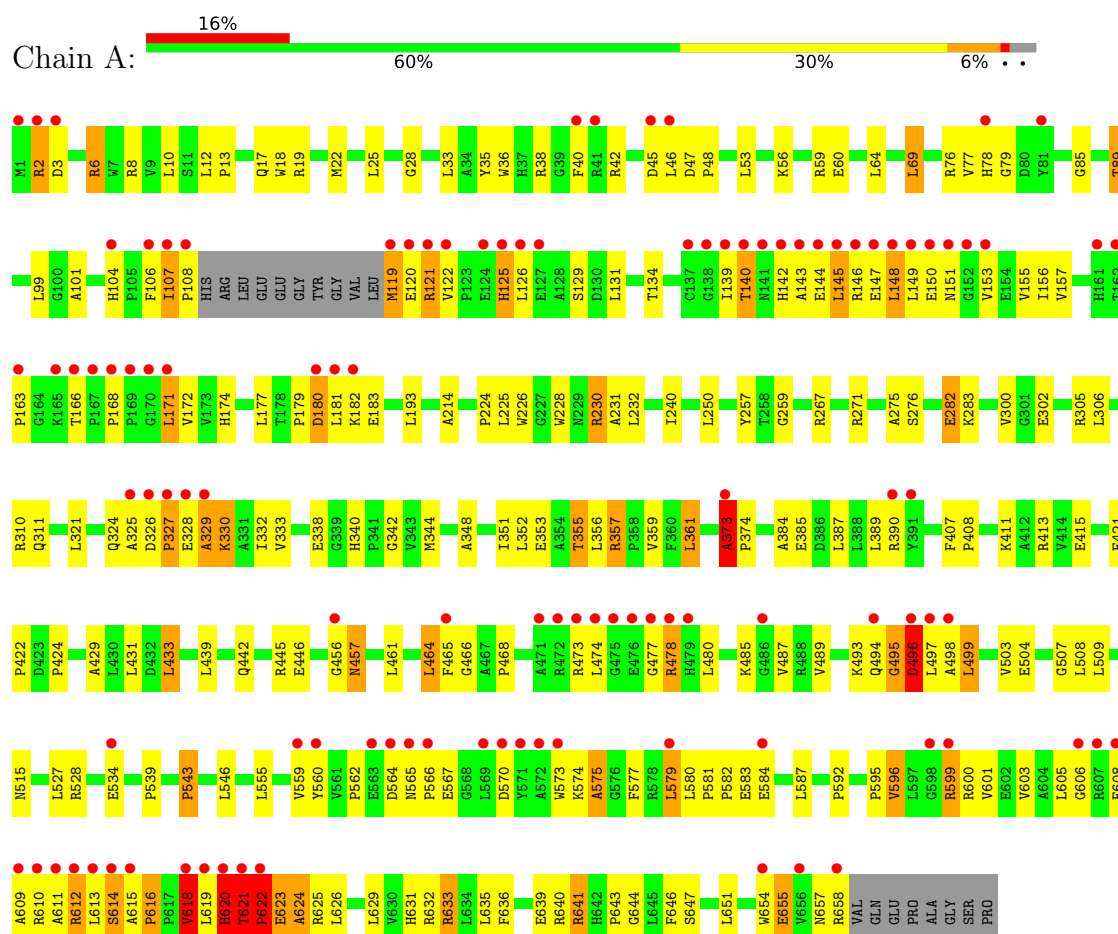
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	293	Total	O	0	0
			293	293		

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	83.13Å 83.13Å 249.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.56 – 2.30 41.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.56-2.30) 99.9 (41.56-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.14 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.281 0.240 , 0.249	Depositor DCC
R_{free} test set	2006 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	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	5315	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: MN

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	0.64	1/5145 (0.0%)	1.08	31/7012 (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	5.71	1.62	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	SER	N-CA-C	-14.85	93.40	113.30
1	A	623	GLU	N-CA-C	-9.61	101.76	112.72
1	A	145	LEU	N-CA-C	-8.76	102.76	113.19
1	A	129	SER	N-CA-C	8.58	122.12	109.07
1	A	155	VAL	N-CA-C	6.93	118.10	108.12
1	A	620	HIS	N-CA-C	6.77	125.22	110.80
1	A	624	ALA	N-CA-C	-6.53	104.00	112.23
1	A	321	LEU	N-CA-C	6.16	120.92	112.04
1	A	373	ALA	CA-C-N	-6.07	113.54	120.89
1	A	373	ALA	C-N-CA	-6.07	113.54	120.89
1	A	329	ALA	N-CA-C	6.05	120.39	112.89
1	A	608	GLU	N-CA-C	-6.00	105.26	113.30
1	A	125	HIS	N-CA-C	-5.77	105.13	111.82
1	A	385	GLU	N-CA-C	5.75	118.29	111.33
1	A	603	VAL	N-CA-C	5.70	116.09	108.11
1	A	230	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	616	PRO	CA-C-N	5.50	125.44	119.78
1	A	616	PRO	C-N-CA	5.50	125.44	119.78
1	A	655	GLU	N-CA-C	5.48	117.26	111.28
1	A	464	LEU	N-CA-C	-5.37	101.81	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	PRO	N-CA-C	5.37	119.52	111.14
1	A	300	VAL	N-CA-C	-5.36	105.15	110.62
1	A	344	MET	N-CA-C	5.33	117.83	111.71
1	A	240	ILE	CB-CA-C	-5.29	108.75	114.35
1	A	507	GLY	N-CA-C	5.28	118.81	111.10
1	A	605	LEU	N-CA-C	-5.11	105.12	112.13
1	A	148	LEU	N-CA-C	-5.09	105.81	111.36
1	A	357	ARG	CA-C-N	-5.04	114.76	119.85
1	A	357	ARG	C-N-CA	-5.04	114.76	119.85
1	A	28	GLY	CA-C-N	5.00	124.61	119.56
1	A	28	GLY	C-N-CA	5.00	124.61	119.56

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	260	0
2	A	2	0	0	0	0
3	A	293	0	0	31	0
All	All	5315	0	5130	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 26.

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:614:SER:HB2	1:A:635:LEU:HD21	1.33	1.11
1:A:276:SER:HB2	3:A:920:HOH:O	1.47	1.10
1:A:126:LEU:HD21	1:A:151:ASN:HB3	1.41	1.03
1:A:182:LYS:HE2	1:A:182:LYS:HA	1.47	0.96
1:A:546:LEU:HD22	1:A:606:GLY:HA2	1.47	0.95
1:A:639:GLU:HB3	3:A:959:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HD22	1:A:606:GLY:CA	1.98	0.93
1:A:643:PRO:O	3:A:961:HOH:O	1.87	0.93
1:A:457:ASN:HD22	1:A:457:ASN:H	0.93	0.91
1:A:621:THR:HG23	1:A:622:PRO:HD3	1.50	0.91
1:A:329:ALA:O	1:A:330:LYS:HB2	1.71	0.90
1:A:457:ASN:HD22	1:A:457:ASN:N	1.64	0.89
1:A:373:ALA:HB1	1:A:374:PRO:CD	2.03	0.89
1:A:620:HIS:O	1:A:622:PRO:HD2	1.74	0.87
1:A:126:LEU:CD2	1:A:151:ASN:HB3	2.04	0.87
1:A:230:ARG:HD2	3:A:671:HOH:O	1.76	0.85
1:A:442:GLN:NE2	1:A:445:ARG:HH21	1.75	0.84
1:A:340:HIS:HD2	1:A:342:GLY:H	1.21	0.83
1:A:592:PRO:HG2	1:A:654:TRP:CH2	2.14	0.83
1:A:328:GLU:HA	3:A:910:HOH:O	1.78	0.82
1:A:107:ILE:HD13	1:A:108:PRO:HD2	1.60	0.82
1:A:457:ASN:H	1:A:457:ASN:ND2	1.76	0.82
1:A:560:TYR:CE2	1:A:582:PRO:HD3	2.14	0.82
1:A:646:PHE:N	3:A:961:HOH:O	2.14	0.81
1:A:565:ASN:CG	1:A:610:ARG:HB2	2.07	0.80
1:A:478:ARG:NH1	1:A:495:GLY:HA2	1.97	0.80
1:A:614:SER:HB2	1:A:635:LEU:CD2	2.11	0.80
1:A:477:GLY:HA3	3:A:861:HOH:O	1.82	0.78
1:A:560:TYR:CD2	1:A:582:PRO:HD3	2.18	0.78
1:A:326:ASP:N	1:A:327:PRO:HD2	2.00	0.77
1:A:546:LEU:HB2	1:A:606:GLY:HA2	1.65	0.77
1:A:85:GLY:O	1:A:89:THR:HG23	1.84	0.76
1:A:565:ASN:ND2	1:A:567:GLU:HB3	2.00	0.76
1:A:179:PRO:O	1:A:180:ASP:HB3	1.85	0.76
1:A:592:PRO:O	1:A:654:TRP:HZ3	1.72	0.73
1:A:17:GLN:HE21	1:A:36:TRP:HE1	1.34	0.73
1:A:107:ILE:HD13	1:A:108:PRO:CD	2.18	0.72
1:A:546:LEU:CD2	1:A:606:GLY:HA2	2.18	0.72
1:A:126:LEU:HD21	1:A:151:ASN:CB	2.18	0.71
1:A:621:THR:HG23	1:A:622:PRO:CD	2.20	0.71
1:A:139:ILE:HG23	1:A:140:THR:HG22	1.73	0.71
1:A:373:ALA:CB	1:A:374:PRO:CD	2.69	0.70
1:A:581:PRO:HG2	1:A:584:GLU:HG2	1.72	0.70
1:A:612:ARG:C	1:A:613:LEU:HD22	2.17	0.70
1:A:442:GLN:HE21	1:A:445:ARG:HH21	1.36	0.70
1:A:144:GLU:C	1:A:146:ARG:H	2.00	0.69
1:A:17:GLN:NE2	1:A:36:TRP:HE1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:H	1:A:327:PRO:HD2	1.55	0.69
1:A:485:LYS:HG3	3:A:955:HOH:O	1.91	0.69
1:A:76:ARG:HE	1:A:104:HIS:HE1	1.40	0.68
1:A:442:GLN:HE21	1:A:445:ARG:NH2	1.91	0.68
1:A:599:ARG:HE	1:A:599:ARG:HA	1.58	0.68
1:A:373:ALA:HB1	1:A:374:PRO:HD2	1.76	0.68
1:A:69:LEU:HD21	1:A:99:LEU:O	1.94	0.68
1:A:478:ARG:HG3	1:A:478:ARG:HH11	1.59	0.68
1:A:559:VAL:HG12	1:A:587:LEU:HD23	1.75	0.67
1:A:592:PRO:HG2	1:A:654:TRP:HH2	1.57	0.67
1:A:351:ILE:O	1:A:355:THR:HB	1.93	0.67
1:A:618:VAL:O	1:A:619:LEU:HD23	1.95	0.67
1:A:327:PRO:O	3:A:910:HOH:O	2.12	0.67
1:A:146:ARG:NH2	1:A:150:GLU:HG2	2.10	0.67
1:A:478:ARG:HH12	1:A:495:GLY:HA2	1.57	0.67
1:A:643:PRO:C	3:A:961:HOH:O	2.35	0.67
1:A:611:ALA:C	1:A:613:LEU:H	2.02	0.66
1:A:622:PRO:O	3:A:958:HOH:O	2.13	0.66
1:A:407:PHE:HB3	1:A:408:PRO:HD3	1.78	0.66
1:A:527:LEU:HD23	1:A:528:ARG:N	2.11	0.65
1:A:146:ARG:O	1:A:150:GLU:N	2.29	0.65
1:A:599:ARG:HB3	1:A:601:VAL:HG13	1.79	0.65
1:A:546:LEU:CB	1:A:606:GLY:HA2	2.28	0.64
1:A:559:VAL:CG1	1:A:587:LEU:HD23	2.27	0.64
1:A:565:ASN:HD21	1:A:567:GLU:HB3	1.60	0.63
1:A:620:HIS:O	1:A:622:PRO:CD	2.45	0.63
1:A:324:GLN:O	1:A:326:ASP:OD1	2.16	0.63
1:A:580:LEU:HD22	1:A:584:GLU:OE1	1.99	0.63
1:A:180:ASP:O	1:A:182:LYS:HE3	1.98	0.63
1:A:621:THR:O	1:A:622:PRO:O	2.17	0.62
1:A:79:GLY:HA3	1:A:89:THR:CG2	2.29	0.62
1:A:411:LYS:O	1:A:415:GLU:HG3	1.99	0.62
1:A:25:LEU:HD13	1:A:46:LEU:HD11	1.81	0.62
1:A:146:ARG:CZ	1:A:150:GLU:HG2	2.29	0.62
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.30	0.62
1:A:76:ARG:NE	1:A:104:HIS:HE1	1.97	0.61
1:A:282:GLU:CD	1:A:282:GLU:H	2.08	0.61
1:A:621:THR:CG2	1:A:622:PRO:HD3	2.28	0.61
1:A:60:GLU:CD	1:A:171:LEU:HD11	2.26	0.60
1:A:613:LEU:HD22	1:A:613:LEU:N	2.17	0.60
1:A:182:LYS:HE2	1:A:182:LYS:CA	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD12	1:A:35:TYR:CD2	2.37	0.59
1:A:230:ARG:CD	3:A:671:HOH:O	2.42	0.59
1:A:497:LEU:O	1:A:498:ALA:HB3	2.02	0.59
1:A:457:ASN:N	1:A:457:ASN:ND2	2.38	0.59
1:A:579:LEU:HD12	3:A:777:HOH:O	2.01	0.59
1:A:613:LEU:HD12	1:A:616:PRO:HD3	1.85	0.59
1:A:142:HIS:CE1	1:A:166:THR:HG23	2.38	0.59
1:A:442:GLN:O	1:A:446:GLU:HG3	2.03	0.59
1:A:613:LEU:CD1	1:A:616:PRO:HD3	2.33	0.58
1:A:324:GLN:O	1:A:326:ASP:N	2.36	0.58
1:A:126:LEU:C	1:A:126:LEU:HD13	2.29	0.57
1:A:373:ALA:HB2	1:A:424:PRO:HB3	1.86	0.57
1:A:629:LEU:C	1:A:629:LEU:HD23	2.29	0.57
1:A:106:PHE:CZ	1:A:121:ARG:HG2	2.39	0.57
1:A:53:LEU:HD21	1:A:183:GLU:HG3	1.85	0.57
1:A:326:ASP:O	1:A:327:PRO:O	2.22	0.57
1:A:373:ALA:HB1	1:A:374:PRO:HD3	1.85	0.57
1:A:144:GLU:C	1:A:146:ARG:N	2.62	0.57
1:A:625:ARG:HD2	3:A:898:HOH:O	2.05	0.57
1:A:13:PRO:HB3	1:A:36:TRP:CD2	2.40	0.57
1:A:373:ALA:CB	1:A:424:PRO:HB3	2.35	0.56
1:A:595:PRO:HD3	1:A:654:TRP:HB3	1.86	0.56
1:A:340:HIS:CD2	1:A:342:GLY:H	2.13	0.56
1:A:76:ARG:HE	1:A:104:HIS:CE1	2.21	0.56
1:A:193:LEU:HD21	1:A:228:TRP:CZ2	2.40	0.56
1:A:583:GLU:HA	1:A:599:ARG:HD2	1.87	0.56
1:A:180:ASP:OD2	1:A:180:ASP:C	2.49	0.55
1:A:340:HIS:HE1	3:A:839:HOH:O	1.89	0.55
1:A:79:GLY:HA3	1:A:89:THR:HG21	1.88	0.55
1:A:104:HIS:HD2	3:A:901:HOH:O	1.90	0.54
1:A:565:ASN:ND2	1:A:610:ARG:HD2	2.22	0.54
1:A:573:TRP:HE3	3:A:935:HOH:O	1.91	0.54
1:A:633:ARG:NH2	3:A:941:HOH:O	2.40	0.54
1:A:647:SER:N	3:A:961:HOH:O	2.09	0.54
1:A:599:ARG:HA	1:A:599:ARG:NE	2.23	0.53
1:A:17:GLN:HE21	1:A:36:TRP:NE1	2.05	0.53
1:A:546:LEU:HD22	1:A:606:GLY:HA3	1.86	0.53
1:A:433:LEU:HD21	1:A:636:PHE:HB2	1.91	0.53
1:A:480:LEU:C	1:A:480:LEU:HD12	2.33	0.53
1:A:651:LEU:HA	1:A:654:TRP:CD1	2.44	0.53
1:A:352:LEU:C	1:A:352:LEU:HD23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:CG	1:A:606:GLY:HA2	2.38	0.52
1:A:302:GLU:OE1	1:A:305:ARG:NH1	2.43	0.52
1:A:611:ALA:C	1:A:613:LEU:N	2.66	0.52
1:A:2:ARG:HD2	1:A:3:ASP:N	2.25	0.52
1:A:355:THR:CG2	1:A:357:ARG:HB2	2.39	0.52
1:A:433:LEU:HD23	1:A:632:ARG:HG2	1.90	0.52
1:A:13:PRO:HB3	1:A:36:TRP:CE3	2.46	0.51
1:A:257:TYR:CZ	1:A:259:GLY:HA2	2.45	0.51
1:A:615:ALA:N	1:A:616:PRO:CD	2.72	0.51
1:A:78:HIS:O	1:A:134:THR:HA	2.10	0.51
1:A:468:PRO:HD3	1:A:503:VAL:HG22	1.93	0.51
1:A:119:MET:HG2	1:A:144:GLU:HG2	1.91	0.51
1:A:478:ARG:HG2	1:A:493:LYS:O	2.11	0.50
1:A:655:GLU:HA	1:A:655:GLU:OE2	2.11	0.50
1:A:473:ARG:HE	1:A:497:LEU:HD22	1.76	0.50
1:A:139:ILE:O	1:A:168:PRO:HD3	2.12	0.50
1:A:53:LEU:CD2	1:A:183:GLU:HG3	2.41	0.50
1:A:69:LEU:CD1	1:A:101:ALA:HB2	2.41	0.50
1:A:565:ASN:C	1:A:567:GLU:H	2.20	0.50
1:A:60:GLU:OE2	1:A:171:LEU:HD21	2.12	0.50
1:A:77:VAL:HG12	1:A:89:THR:HB	1.94	0.50
1:A:461:LEU:HD23	1:A:508:LEU:HD23	1.94	0.49
1:A:496:ASP:O	1:A:497:LEU:HB2	2.12	0.49
1:A:560:TYR:OH	1:A:592:PRO:HA	2.12	0.49
1:A:565:ASN:C	1:A:567:GLU:N	2.64	0.49
1:A:612:ARG:O	1:A:612:ARG:HG2	2.13	0.49
1:A:38:ARG:HH11	1:A:457:ASN:HB2	1.78	0.48
1:A:267:ARG:O	1:A:271:ARG:HD3	2.13	0.48
1:A:478:ARG:CZ	1:A:495:GLY:HA2	2.42	0.48
1:A:515:ASN:CG	1:A:515:ASN:O	2.56	0.48
1:A:565:ASN:HB2	3:A:915:HOH:O	2.12	0.48
1:A:478:ARG:HH11	1:A:478:ARG:CG	2.26	0.48
1:A:139:ILE:CG2	1:A:140:THR:HG22	2.42	0.48
1:A:527:LEU:HD23	1:A:527:LEU:C	2.39	0.48
1:A:147:GLU:HB2	1:A:153:VAL:HB	1.95	0.47
1:A:332:ILE:HD12	1:A:355:THR:HG21	1.96	0.47
1:A:48:PRO:HG2	1:A:231:ALA:HB2	1.96	0.47
1:A:226:TRP:CD1	3:A:925:HOH:O	2.66	0.47
1:A:348:ALA:HB2	1:A:361:LEU:HD22	1.96	0.47
1:A:76:ARG:NH1	1:A:125:HIS:HD2	2.12	0.47
1:A:573:TRP:C	1:A:575:ALA:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ARG:O	1:A:613:LEU:HB2	2.14	0.47
1:A:389:LEU:C	1:A:390:ARG:HG3	2.40	0.47
1:A:592:PRO:O	1:A:654:TRP:CZ3	2.61	0.47
1:A:149:LEU:HD23	1:A:150:GLU:N	2.29	0.47
1:A:77:VAL:CG1	1:A:89:THR:HB	2.45	0.47
1:A:79:GLY:HA3	1:A:89:THR:HG22	1.96	0.47
1:A:543:PRO:HB2	1:A:641:ARG:HA	1.97	0.47
1:A:326:ASP:O	1:A:327:PRO:C	2.57	0.47
1:A:565:ASN:N	1:A:566:PRO:HD3	2.29	0.47
1:A:611:ALA:O	1:A:613:LEU:N	2.48	0.47
1:A:338:GLU:HB2	3:A:887:HOH:O	2.14	0.46
1:A:465:PHE:CD2	1:A:504:GLU:HG3	2.50	0.46
1:A:644:GLY:C	3:A:961:HOH:O	2.58	0.46
1:A:12:LEU:HD22	1:A:18:TRP:CH2	2.51	0.46
1:A:131:LEU:HD11	1:A:156:ILE:HG13	1.98	0.46
1:A:311:GLN:HG2	3:A:952:HOH:O	2.15	0.46
1:A:473:ARG:HG2	1:A:474:LEU:N	2.31	0.46
1:A:494:GLN:O	1:A:495:GLY:C	2.58	0.46
1:A:174:HIS:HB3	1:A:177:LEU:HG	1.98	0.46
1:A:581:PRO:CG	1:A:584:GLU:HG2	2.45	0.46
1:A:613:LEU:N	1:A:613:LEU:CD2	2.78	0.46
1:A:142:HIS:CE1	1:A:166:THR:O	2.69	0.46
1:A:134:THR:OG1	1:A:157:VAL:HA	2.15	0.45
1:A:310:ARG:NH1	3:A:952:HOH:O	2.49	0.45
1:A:480:LEU:HD21	1:A:493:LYS:HB2	1.97	0.45
1:A:565:ASN:OD1	1:A:610:ARG:HB2	2.16	0.45
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.81	0.45
1:A:6:ARG:HB3	1:A:534:GLU:OE1	2.16	0.45
1:A:119:MET:HA	1:A:122:VAL:HG23	1.97	0.45
1:A:566:PRO:O	1:A:570:ASP:N	2.50	0.45
1:A:478:ARG:NH1	1:A:478:ARG:HG3	2.29	0.45
1:A:64:LEU:HD22	1:A:171:LEU:HD23	1.99	0.45
1:A:224:PRO:HB3	1:A:226:TRP:CH2	2.52	0.45
1:A:493:LYS:HG2	1:A:497:LEU:CA	2.47	0.45
1:A:493:LYS:HG2	1:A:497:LEU:HA	1.98	0.45
1:A:600:ARG:NH1	3:A:914:HOH:O	2.49	0.45
1:A:142:HIS:HE1	1:A:166:THR:O	1.99	0.44
1:A:565:ASN:HD22	1:A:610:ARG:HD2	1.82	0.44
1:A:622:PRO:C	1:A:624:ALA:H	2.24	0.44
1:A:622:PRO:C	3:A:958:HOH:O	2.60	0.44
1:A:635:LEU:O	1:A:639:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:H	1:A:456:GLY:N	2.15	0.44
1:A:478:ARG:NH1	1:A:478:ARG:CG	2.81	0.44
1:A:595:PRO:HA	1:A:654:TRP:CE2	2.52	0.44
1:A:559:VAL:HG12	1:A:587:LEU:CD2	2.45	0.44
1:A:631:HIS:O	1:A:635:LEU:HD23	2.17	0.44
1:A:465:PHE:CD1	1:A:466:GLY:N	2.86	0.43
1:A:38:ARG:HB2	1:A:40:PHE:CD1	2.53	0.43
1:A:40:PHE:CE2	1:A:45:ASP:O	2.71	0.43
1:A:19:ARG:HA	1:A:22:MET:HE3	2.01	0.43
1:A:464:LEU:HD12	1:A:464:LEU:N	2.34	0.43
1:A:655:GLU:OE1	1:A:658:ARG:NH2	2.52	0.43
1:A:497:LEU:O	1:A:498:ALA:CB	2.67	0.43
1:A:172:VAL:HG13	1:A:172:VAL:O	2.17	0.43
1:A:615:ALA:N	1:A:616:PRO:HD2	2.33	0.43
1:A:625:ARG:HG3	3:A:958:HOH:O	2.18	0.43
1:A:496:ASP:C	1:A:497:LEU:O	2.60	0.43
1:A:143:ALA:C	1:A:145:LEU:H	2.27	0.42
1:A:421:PHE:HB3	1:A:422:PRO:HD2	2.00	0.42
1:A:596:VAL:HG12	1:A:599:ARG:CG	2.48	0.42
1:A:641:ARG:O	1:A:643:PRO:HD3	2.19	0.42
1:A:655:GLU:C	1:A:657:ASN:H	2.27	0.42
1:A:384:ALA:HB2	1:A:413:ARG:HG2	2.02	0.42
1:A:85:GLY:O	1:A:89:THR:CG2	2.62	0.42
1:A:180:ASP:O	1:A:181:LEU:C	2.62	0.42
1:A:17:GLN:NE2	1:A:36:TRP:NE1	2.64	0.42
1:A:442:GLN:NE2	1:A:445:ARG:NH2	2.50	0.42
1:A:493:LYS:HG2	1:A:497:LEU:H	1.85	0.42
1:A:275:ALA:HA	1:A:306:LEU:HD13	2.02	0.42
1:A:646:PHE:CA	3:A:961:HOH:O	2.65	0.42
1:A:613:LEU:HD13	1:A:613:LEU:HA	1.47	0.42
1:A:38:ARG:HB2	1:A:40:PHE:HD1	1.85	0.42
1:A:8:ARG:NH2	1:A:534:GLU:OE2	2.52	0.41
1:A:10:LEU:HD21	1:A:429:ALA:HB1	2.02	0.41
1:A:225:LEU:H	1:A:456:GLY:H	1.68	0.41
1:A:635:LEU:HD22	1:A:635:LEU:N	2.35	0.41
1:A:59:ARG:NH1	3:A:817:HOH:O	2.54	0.41
1:A:493:LYS:CG	1:A:497:LEU:H	2.33	0.41
1:A:333:VAL:HB	1:A:411:LYS:HG3	2.01	0.41
1:A:38:ARG:NH1	1:A:457:ASN:HB2	2.34	0.41
1:A:606:GLY:HA3	1:A:609:ALA:CB	2.50	0.41
1:A:577:PHE:HB2	1:A:579:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:N	1:A:499:LEU:HD22	2.37	0.40
1:A:581:PRO:HB2	1:A:583:GLU:OE2	2.20	0.40
1:A:214:ALA:HB1	1:A:232:LEU:HD21	2.02	0.40
1:A:359:VAL:HG12	1:A:361:LEU:HD13	2.03	0.40
1:A:562:PRO:HG2	3:A:728:HOH:O	2.22	0.40
1:A:143:ALA:O	1:A:145:LEU:HD23	2.21	0.40
1:A:329:ALA:O	1:A:330:LYS:CB	2.52	0.40
1:A:493:LYS:HZ2	1:A:496:ASP:HB2	1.87	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%)	589 (92%)	39 (6%)	16 (2%)	4 3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	622	PRO
1	A	495	GLY
1	A	612	ARG
1	A	618	VAL
1	A	163	PRO
1	A	180	ASP
1	A	330	LYS

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Mol	Chain	Res	Type
1	A	575	ALA
1	A	574	LYS
1	A	596	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%)	457 (91%)	45 (9%)	9 12

All (45) 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	47	ASP
1	A	56	LYS
1	A	69	LEU
1	A	89	THR
1	A	107	ILE
1	A	119	MET
1	A	120	GLU
1	A	121	ARG
1	A	140	THR
1	A	148	LEU
1	A	171	LEU
1	A	250	LEU
1	A	282	GLU
1	A	283	LYS
1	A	353	GLU
1	A	355	THR
1	A	356	LEU
1	A	361	LEU
1	A	387	LEU
1	A	431	LEU

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Mol	Chain	Res	Type
1	A	433	LEU
1	A	439	LEU
1	A	457	ASN
1	A	478	ARG
1	A	487	VAL
1	A	489	VAL
1	A	496	ASP
1	A	499	LEU
1	A	509	LEU
1	A	543	PRO
1	A	555	LEU
1	A	564	ASP
1	A	579	LEU
1	A	599	ARG
1	A	618	VAL
1	A	621	THR
1	A	622	PRO
1	A	623	GLU
1	A	626	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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	71	GLN
1	A	104	HIS
1	A	141	ASN
1	A	142	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	479	HIS
1	A	494	GLN
1	A	565	ASN

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 2 ligands modelled in this entry, 2 are 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	648/666 (97%)	0.73	109 (16%) 4 5	13, 32, 67, 78	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	THR	7.5
1	A	1	MET	6.1
1	A	618	VAL	6.1
1	A	619	LEU	5.7
1	A	613	LEU	5.6
1	A	477	GLY	5.6
1	A	149	LEU	5.5
1	A	325	ALA	5.3
1	A	609	ALA	5.1
1	A	148	LEU	5.0
1	A	606	GLY	5.0
1	A	607	ARG	4.5
1	A	162	THR	4.5
1	A	145	LEU	4.5
1	A	608	GLU	4.2
1	A	327	PRO	4.2
1	A	107	ILE	4.0
1	A	138	GLY	4.0
1	A	456	GLY	4.0
1	A	615	ALA	3.9
1	A	167	PRO	3.8
1	A	147	GLU	3.7
1	A	119	MET	3.7
1	A	140	THR	3.7
1	A	598	GLY	3.7
1	A	326	ASP	3.7
1	A	565	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	566	PRO	3.5
1	A	161	HIS	3.5
1	A	143	ALA	3.4
1	A	475	GLY	3.4
1	A	569	LEU	3.4
1	A	139	ILE	3.4
1	A	108	PRO	3.4
1	A	599	ARG	3.4
1	A	137	CYS	3.4
1	A	150	GLU	3.3
1	A	654	TRP	3.2
1	A	151	ASN	3.2
1	A	126	LEU	3.2
1	A	622	PRO	3.1
1	A	584	GLU	3.1
1	A	40	PHE	3.1
1	A	474	LEU	3.1
1	A	127	GLU	3.1
1	A	166	THR	3.1
1	A	144	GLU	3.0
1	A	534	GLU	3.0
1	A	122	VAL	3.0
1	A	163	PRO	3.0
1	A	610	ARG	2.9
1	A	573	TRP	2.9
1	A	146	ARG	2.9
1	A	611	ALA	2.9
1	A	168	PRO	2.8
1	A	472	ARG	2.8
1	A	171	LEU	2.8
1	A	479	HIS	2.8
1	A	2	ARG	2.8
1	A	78	HIS	2.7
1	A	81	TYR	2.7
1	A	571	TYR	2.7
1	A	494	GLN	2.7
1	A	169	PRO	2.7
1	A	46	LEU	2.7
1	A	373	ALA	2.6
1	A	141	ASN	2.6
1	A	106	PHE	2.6
1	A	142	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	497	LEU	2.5
1	A	41	ARG	2.5
1	A	180	ASP	2.5
1	A	120	GLU	2.5
1	A	476	GLU	2.5
1	A	559	VAL	2.5
1	A	614	SER	2.5
1	A	478	ARG	2.4
1	A	656	VAL	2.4
1	A	121	ARG	2.4
1	A	612	ARG	2.4
1	A	498	ALA	2.4
1	A	658	ARG	2.4
1	A	104	HIS	2.3
1	A	564	ASP	2.3
1	A	125	HIS	2.3
1	A	560	TYR	2.3
1	A	165	LYS	2.3
1	A	572	ALA	2.2
1	A	620	HIS	2.2
1	A	579	LEU	2.2
1	A	390	ARG	2.2
1	A	570	ASP	2.2
1	A	152	GLY	2.2
1	A	486	GLY	2.2
1	A	471	ALA	2.2
1	A	473	ARG	2.1
1	A	124	GLU	2.1
1	A	153	VAL	2.1
1	A	182	LYS	2.1
1	A	181	LEU	2.1
1	A	45	ASP	2.1
1	A	170	GLY	2.1
1	A	391	TYR	2.1
1	A	465	PHE	2.1
1	A	328	GLU	2.0
1	A	329	ALA	2.0
1	A	563	GLU	2.0
1	A	3	ASP	2.0
1	A	496	ASP	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](#)

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	MN	A	668	1/1	0.96	0.14	65,65,65,65	0
2	MN	A	667	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.