WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 08:06 PM EST

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PDB ID	:	4RO1
Title	:	An 3'-5'-exoribonuclease that specifically recognizes RNAs.
Authors	:	Lv, H.; Zhu, Y.; Teng, M.
Deposited on	:	2014-10-27
Resolution	:	2.80 Å(reported)

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 2.80 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.

| ∎ Percentile relative to all X-ray structures |
| ⬚ Percentile relative to X-ray structures of similar resolution |
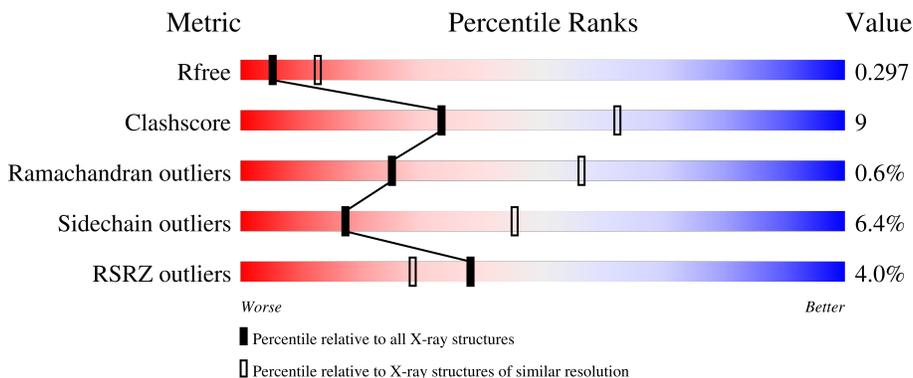
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	764	4% / 60% 13% • 26%
1	B	764	2% / 57% 16% • 26%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8275 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 DIS3-like exonuclease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	568	Total	C	N	O	S	0	0	0
			4193	2647	723	805	18			
1	A	566	Total	C	N	O	S	0	0	0
			4082	2583	710	770	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	HIS	-	expression tag	UNP O14040
A	165	HIS	-	expression tag	UNP O14040
A	166	HIS	-	expression tag	UNP O14040
A	167	HIS	-	expression tag	UNP O14040
A	168	HIS	-	expression tag	UNP O14040
A	169	HIS	-	expression tag	UNP O14040
B	164	HIS	-	expression tag	UNP O14040
B	165	HIS	-	expression tag	UNP O14040
B	166	HIS	-	expression tag	UNP O14040
B	167	HIS	-	expression tag	UNP O14040
B	168	HIS	-	expression tag	UNP O14040
B	169	HIS	-	expression tag	UNP O14040

3 Residue-property plots ⓘ

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: DIS3-like exonuclease 2

Chain B:

• Molecule 1: DIS3-like exonuclease 2

Chain A:
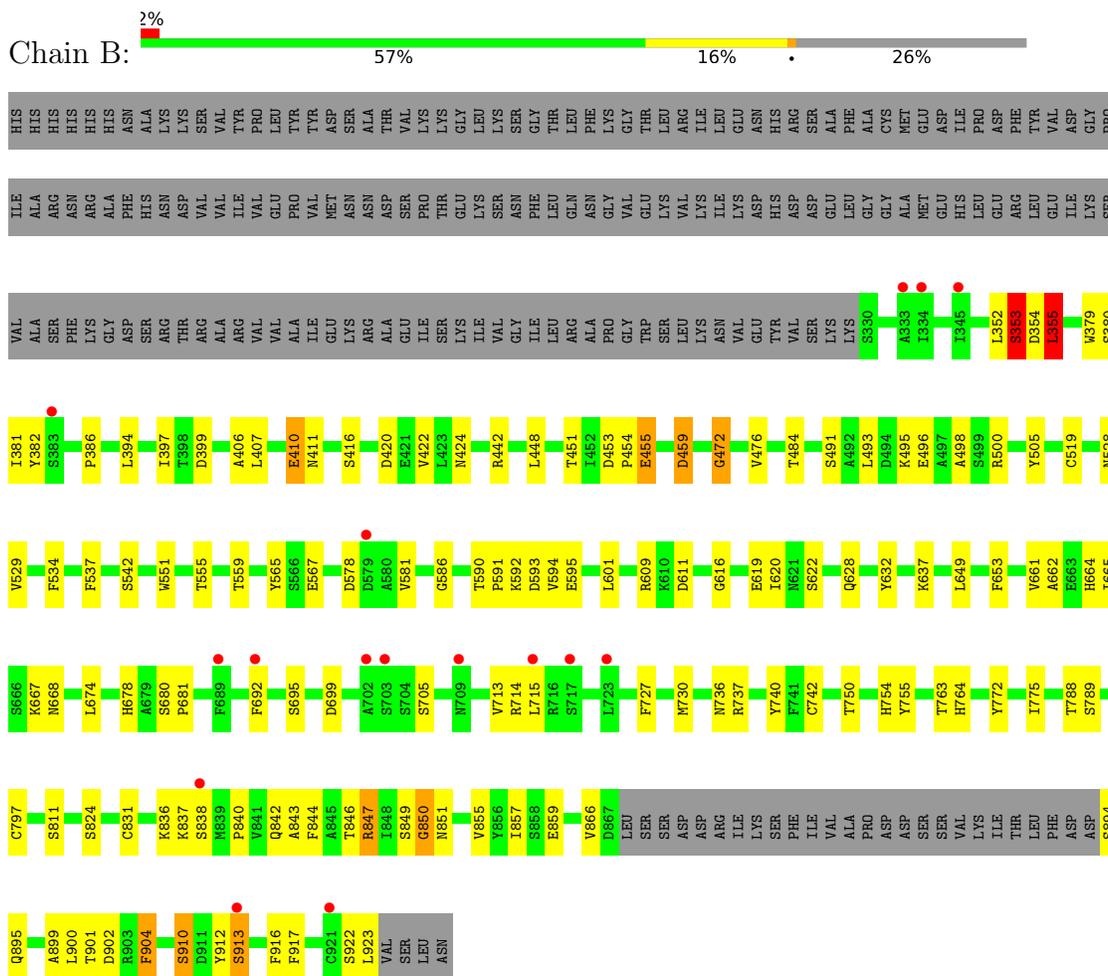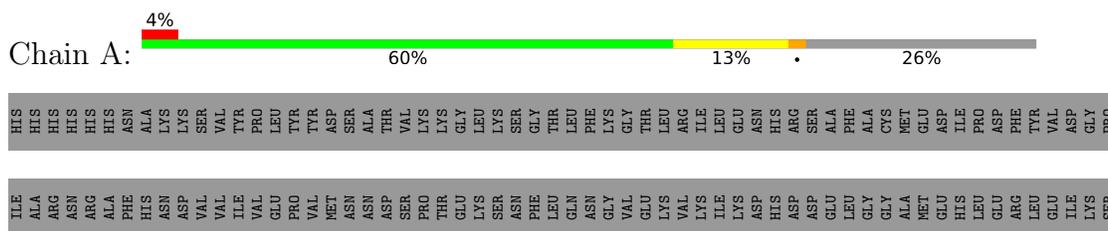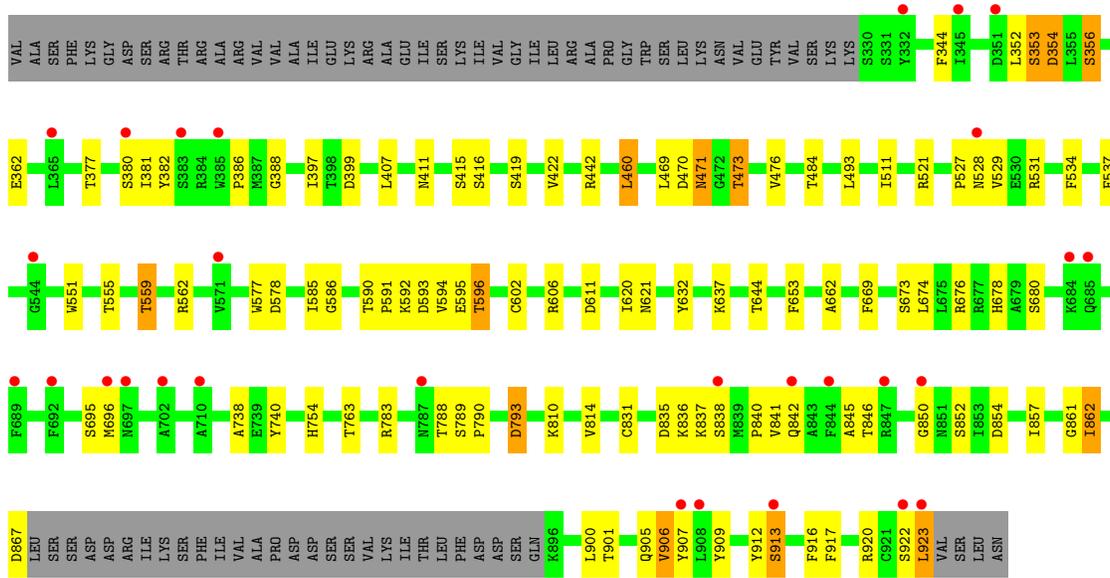
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	116.97Å 54.20Å 127.22Å 90.00° 107.09° 90.00°	Depositor
Resolution (Å)	40.53 – 2.80	Depositor
	40.53 – 2.80	EDS
% Data completeness (in resolution range)	99.4 (40.53-2.80)	Depositor
	99.5 (40.53-2.80)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.269 , 0.294	Depositor
	0.283 , 0.297	DCC
R_{free} test set	1890 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8275	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.31	0/4174	0.60	4/5700 (0.1%)
1	B	0.32	0/4284	0.62	6/5840 (0.1%)
All	All	0.32	0/8458	0.61	10/11540 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	356	SER	N-CA-CB	-5.84	101.74	110.50
1	A	837	LYS	N-CA-C	5.82	126.70	111.00
1	A	470	ASP	CB-CA-C	-5.70	99.00	110.40
1	B	353	SER	N-CA-CB	5.65	118.98	110.50
1	B	847	ARG	N-CA-CB	-5.65	100.44	110.60
1	A	621	ASN	N-CA-CB	-5.60	100.51	110.60
1	B	455	GLU	CB-CA-C	-5.54	99.33	110.40
1	B	355	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	472	GLY	N-CA-C	-5.20	100.11	113.10
1	B	837	LYS	N-CA-CB	-5.02	101.56	110.60

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	4082	0	3570	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4193	0	3765	75	0
All	All	8275	0	7335	134	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 9.

All (134) 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:831:CYS:HB3	1:A:836:LYS:O	1.50	1.12
1:A:352:LEU:HB2	1:A:356:SER:CB	1.88	1.02
1:B:353:SER:OG	1:B:353:SER:O	1.80	0.90
1:B:353:SER:O	1:B:354:ASP:OD1	1.93	0.84
1:B:590:THR:HG22	1:B:592:LYS:H	1.44	0.80
1:A:840:PRO:HG2	1:A:906:VAL:HG23	1.70	0.74
1:B:394:LEU:HD13	1:B:397:ILE:HD12	1.69	0.74
1:B:788:THR:HG22	1:B:789:SER:H	1.53	0.72
1:A:788:THR:HG22	1:A:789:SER:H	1.54	0.72
1:B:699:ASP:O	1:B:714:ARG:NH2	2.22	0.72
1:A:838:SER:O	1:A:840:PRO:HD3	1.90	0.72
1:B:913:SER:N	1:B:916:PHE:O	2.23	0.71
1:A:602:CYS:SG	1:A:606:ARG:NH1	2.65	0.70
1:B:397:ILE:HD11	1:B:632:TYR:HB3	1.73	0.70
1:B:420:ASP:O	1:B:424:ASN:ND2	2.20	0.69
1:B:567:GLU:HB3	1:B:581:VAL:HG22	1.75	0.69
1:B:846:THR:H	1:B:847:ARG:HA	1.58	0.68
1:B:484:THR:HG22	1:B:775:ILE:HG23	1.76	0.67
1:B:454:PRO:O	1:B:455:GLU:CB	2.42	0.67
1:A:442:ARG:HB3	1:A:555:THR:HG22	1.76	0.67
1:A:913:SER:N	1:A:916:PHE:O	2.27	0.66
1:A:527:PRO:HA	1:A:559:THR:HG22	1.77	0.66
1:B:399:ASP:HB3	1:B:913:SER:HB3	1.78	0.65
1:B:727:PHE:HA	1:B:730:MET:HE2	1.79	0.65
1:B:451:THR:HG23	1:B:559:THR:HG21	1.79	0.64
1:A:793:ASP:OD1	1:A:793:ASP:N	2.32	0.63
1:A:845:ALA:O	1:A:900:LEU:HA	1.98	0.63
1:A:521:ARG:O	1:A:531:ARG:NE	2.32	0.62
1:B:850:GLY:CA	1:B:851:ASN:HB2	2.30	0.61
1:B:831:CYS:HB3	1:B:836:LYS:O	2.01	0.60
1:A:831:CYS:CB	1:A:836:LYS:O	2.40	0.59
1:B:678:HIS:NE2	1:B:736:ASN:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:VAL:HA	1:A:905:GLN:HA	1.86	0.58
1:A:407:LEU:O	1:A:411:ASN:ND2	2.33	0.57
1:B:591:PRO:O	1:B:595:GLU:HG3	2.05	0.57
1:B:628:GLN:HB3	1:B:637:LYS:HB2	1.85	0.57
1:A:469:LEU:HD12	1:A:473:THR:HG22	1.86	0.57
1:B:846:THR:N	1:B:847:ARG:HA	2.21	0.56
1:A:577:TRP:O	1:A:577:TRP:CD1	2.58	0.56
1:A:678:HIS:H	1:A:754:HIS:HA	1.71	0.55
1:A:842:GLN:O	1:A:857:ILE:HA	2.07	0.55
1:B:353:SER:O	1:B:354:ASP:CG	2.45	0.55
1:B:894:SER:O	1:B:895:GLN:HB2	2.07	0.55
1:A:912:TYR:HD1	1:A:913:SER:HB2	1.72	0.54
1:B:442:ARG:HB3	1:B:555:THR:HG22	1.89	0.54
1:B:850:GLY:HA3	1:B:851:ASN:CB	2.38	0.53
1:B:399:ASP:HB3	1:B:913:SER:CB	2.38	0.53
1:B:678:HIS:H	1:B:754:HIS:HA	1.74	0.53
1:B:674:LEU:HD11	1:B:740:TYR:HB3	1.90	0.53
1:B:681:PRO:HD3	1:B:755:TYR:CE1	2.44	0.53
1:B:922:SER:OG	1:B:923:LEU:N	2.40	0.53
1:A:674:LEU:HD11	1:A:740:TYR:HB3	1.90	0.52
1:A:912:TYR:CD1	1:A:913:SER:HB2	2.45	0.52
1:B:857:ILE:O	1:B:859:GLU:O	2.28	0.51
1:B:900:LEU:O	1:B:901:THR:CB	2.57	0.51
1:A:669:PHE:O	1:A:673:SER:OG	2.20	0.51
1:B:422:VAL:HG13	1:B:493:LEU:HA	1.93	0.50
1:B:850:GLY:HA3	1:B:851:ASN:HB2	1.92	0.50
1:B:912:TYR:HD1	1:B:913:SER:HB2	1.76	0.50
1:A:922:SER:OG	1:A:923:LEU:N	2.45	0.50
1:B:601:LEU:HB3	1:B:649:LEU:HD21	1.94	0.50
1:A:399:ASP:HB3	1:A:913:SER:HB3	1.93	0.50
1:A:592:LYS:O	1:A:596:THR:HG22	2.11	0.50
1:B:476:VAL:HG11	1:B:653:PHE:CE1	2.47	0.49
1:A:399:ASP:O	1:A:913:SER:OG	2.28	0.48
1:B:453:ASP:HB3	1:B:454:PRO:HD2	1.94	0.48
1:A:344:PHE:O	1:A:386:PRO:HD2	2.13	0.48
1:A:422:VAL:HG13	1:A:493:LEU:HA	1.94	0.48
1:A:662:ALA:HB2	1:A:763:THR:HG22	1.95	0.48
1:B:866:VAL:HG23	1:B:922:SER:HA	1.96	0.48
1:A:590:THR:H	1:A:593:ASP:HB2	1.79	0.48
1:B:838:SER:O	1:B:840:PRO:HD3	2.13	0.47
1:A:476:VAL:HG11	1:A:653:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:CYS:CB	1:B:797:CYS:SG	3.02	0.47
1:B:824:SER:O	1:B:910:SER:OG	2.26	0.47
1:B:406:ALA:O	1:B:410:GLU:HG3	2.14	0.47
1:B:664:HIS:HA	1:B:667:LYS:HE2	1.96	0.47
1:A:669:PHE:CD1	1:A:790:PRO:HG3	2.50	0.47
1:B:692:PHE:CE1	1:B:730:MET:HE1	2.50	0.47
1:A:900:LEU:O	1:A:901:THR:CB	2.62	0.47
1:A:861:GLY:O	1:A:862:ILE:CB	2.63	0.46
1:A:353:SER:HB3	1:A:354:ASP:H	1.41	0.46
1:A:585:ILE:HD13	1:A:594:VAL:HG21	1.97	0.46
1:A:469:LEU:O	1:A:471:ASN:O	2.34	0.46
1:A:850:GLY:HA2	1:A:852:SER:H	1.81	0.46
1:B:496:GLU:O	1:B:500:ARG:HG3	2.15	0.46
1:A:537:PHE:HB2	1:A:551:TRP:HB3	1.97	0.46
1:B:904:PHE:N	1:B:904:PHE:CD1	2.83	0.46
1:B:912:TYR:CD1	1:B:913:SER:HB2	2.51	0.46
1:A:846:THR:O	1:A:854:ASP:O	2.34	0.46
1:B:537:PHE:HB2	1:B:551:TRP:HB3	1.98	0.45
1:B:736:ASN:OD1	1:B:737:ARG:N	2.47	0.45
1:A:460:LEU:HD11	1:A:562:ARG:HD2	1.99	0.45
1:B:454:PRO:HA	1:B:565:TYR:HD2	1.81	0.45
1:B:899:ALA:O	1:B:902:ASP:OD1	2.35	0.45
1:B:850:GLY:CA	1:B:851:ASN:CB	2.96	0.44
1:B:843:ALA:HB3	1:B:904:PHE:O	2.18	0.43
1:A:399:ASP:HB3	1:A:913:SER:CB	2.47	0.43
1:A:528:ASN:OD1	1:A:586:GLY:HA3	2.17	0.43
1:B:380:SER:C	1:B:382:TYR:H	2.21	0.43
1:B:459:ASP:OD2	1:B:505:TYR:OH	2.31	0.43
1:A:527:PRO:HG3	1:A:562:ARG:HB2	1.99	0.43
1:A:810:LYS:O	1:A:814:VAL:HG13	2.18	0.43
1:A:415:SER:HB2	1:A:511:ILE:HD12	2.01	0.43
1:A:912:TYR:HA	1:A:917:PHE:HA	2.00	0.43
1:B:352:LEU:O	1:B:355:LEU:HB2	2.18	0.42
1:B:498:ALA:HB2	1:B:772:TYR:CZ	2.54	0.42
1:A:397:ILE:HD11	1:A:632:TYR:HB3	2.01	0.42
1:B:491:SER:O	1:B:495:LYS:HG3	2.18	0.42
1:A:380:SER:C	1:A:382:TYR:H	2.23	0.42
1:A:835:ASP:O	1:A:836:LYS:C	2.58	0.42
1:A:591:PRO:O	1:A:595:GLU:HG3	2.19	0.42
1:A:676:ARG:NH2	1:A:738:ALA:HB3	2.34	0.42
1:B:590:THR:H	1:B:593:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:VAL:HB	1:A:907:TYR:H	1.67	0.42
1:B:397:ILE:CD1	1:B:632:TYR:HB3	2.45	0.42
1:A:377:THR:HG23	1:A:388:GLY:HA2	2.01	0.42
1:B:912:TYR:HA	1:B:917:PHE:HA	2.02	0.42
1:B:448:LEU:HD21	1:B:594:VAL:HG22	2.01	0.41
1:A:909:TYR:N	1:A:920:ARG:O	2.43	0.41
1:B:407:LEU:O	1:B:411:ASN:ND2	2.49	0.41
1:B:661:VAL:O	1:B:665:ILE:HG12	2.20	0.41
1:B:662:ALA:HB2	1:B:763:THR:HG22	2.03	0.41
1:B:616:GLY:O	1:B:705:SER:HB3	2.20	0.41
1:B:410:GLU:HG3	1:B:410:GLU:H	1.67	0.41
1:A:471:ASN:OD1	1:A:471:ASN:N	2.52	0.41
1:B:842:GLN:O	1:B:857:ILE:HA	2.21	0.41
1:B:379:TRP:CZ2	1:B:386:PRO:HD3	2.55	0.40
1:B:528:ASN:OD1	1:B:586:GLY:HA3	2.20	0.40
1:B:763:THR:OG1	1:B:764:HIS:N	2.54	0.40
1:B:846:THR:N	1:B:847:ARG:CA	2.84	0.40
1:B:844:PHE:O	1:B:855:VAL:HA	2.22	0.40
1:A:783:ARG:HD3	1:A:789:SER:O	2.21	0.40
1:A:788:THR:HG22	1:A:789:SER:N	2.31	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	562/764 (74%)	494 (88%)	65 (12%)	3 (0%)	29	61
1	B	564/764 (74%)	487 (86%)	73 (13%)	4 (1%)	22	53
All	All	1126/1528 (74%)	981 (87%)	138 (12%)	7 (1%)	25	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	850	GLY
1	A	354	ASP
1	B	381	ILE
1	B	472	GLY
1	A	862	ILE
1	B	620	ILE
1	A	381	ILE

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	373/683 (55%)	348 (93%)	25 (7%)	16	43
1	B	406/683 (59%)	381 (94%)	25 (6%)	18	47
All	All	779/1366 (57%)	729 (94%)	50 (6%)	17	45

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	353	SER
1	B	355	LEU
1	B	410	GLU
1	B	416	SER
1	B	459	ASP
1	B	519	CYS
1	B	529	VAL
1	B	534	PHE
1	B	542	SER
1	B	578	ASP
1	B	609	ARG
1	B	611	ASP
1	B	619	GLU
1	B	622	SER
1	B	668	ASN
1	B	680	SER
1	B	695	SER

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
1	B	713	VAL
1	B	715	LEU
1	B	750	THR
1	B	811	SER
1	B	849	SER
1	B	904	PHE
1	B	910	SER
1	B	913	SER
1	A	353	SER
1	A	362	GLU
1	A	416	SER
1	A	419	SER
1	A	460	LEU
1	A	471	ASN
1	A	473	THR
1	A	484	THR
1	A	529	VAL
1	A	534	PHE
1	A	559	THR
1	A	578	ASP
1	A	596	THR
1	A	611	ASP
1	A	620	ILE
1	A	637	LYS
1	A	644	THR
1	A	680	SER
1	A	695	SER
1	A	696	MET
1	A	793	ASP
1	A	867	ASP
1	A	906	VAL
1	A	913	SER
1	A	923	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	566/764 (74%)	0.27	29 (5%)	28	19	41, 66, 94, 109	0
1	B	568/764 (74%)	0.09	16 (2%)	53	43	28, 50, 91, 103	0
All	All	1134/1528 (74%)	0.18	45 (3%)	38	28	28, 59, 93, 109	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	TRP	5.7
1	B	703	SER	4.3
1	A	838	SER	3.9
1	A	787	ASN	3.5
1	B	689	PHE	3.3
1	A	692	PHE	3.2
1	B	702	ALA	3.2
1	A	702	ALA	3.2
1	A	351	ASP	3.1
1	A	923	LEU	3.0
1	A	365	LEU	3.0
1	A	697	ASN	2.9
1	B	383	SER	2.9
1	A	922	SER	2.9
1	B	723	LEU	2.8
1	A	383	SER	2.8
1	A	380	SER	2.8
1	B	717	SER	2.8
1	A	685	GLN	2.7
1	B	715	LEU	2.6
1	A	689	PHE	2.5
1	A	345	ILE	2.5
1	B	334	ILE	2.4
1	A	332	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	696	MET	2.3
1	B	838	SER	2.3
1	B	345	ILE	2.3
1	A	908	LEU	2.3
1	A	850	GLY	2.3
1	A	710	ALA	2.3
1	B	579	ASP	2.2
1	A	913	SER	2.2
1	A	684	LYS	2.2
1	A	844	PHE	2.2
1	A	571	VAL	2.2
1	A	528	ASN	2.2
1	B	333	ALA	2.2
1	B	913	SER	2.2
1	B	709	ASN	2.1
1	A	842	GLN	2.1
1	A	847	ARG	2.1
1	B	921	CYS	2.1
1	A	544	GLY	2.1
1	A	907	TYR	2.0
1	B	692	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.