



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:38 AM UTC

PDB ID : 4RO1 / pdb_00004ro1
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)

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

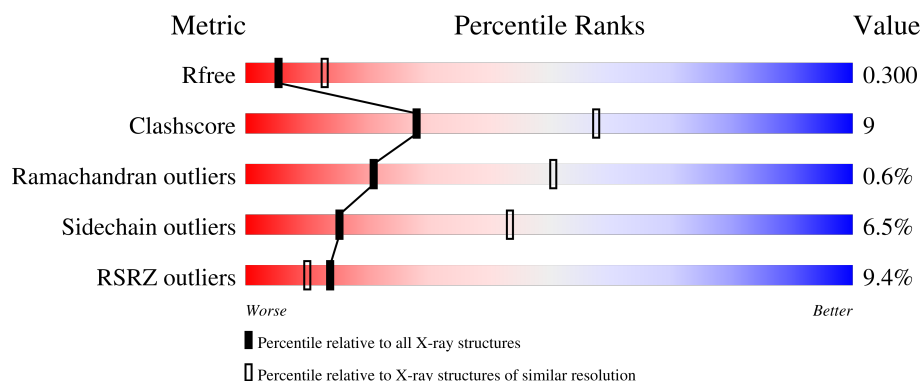
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	764	
1	B	764	

2 Entry composition

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			

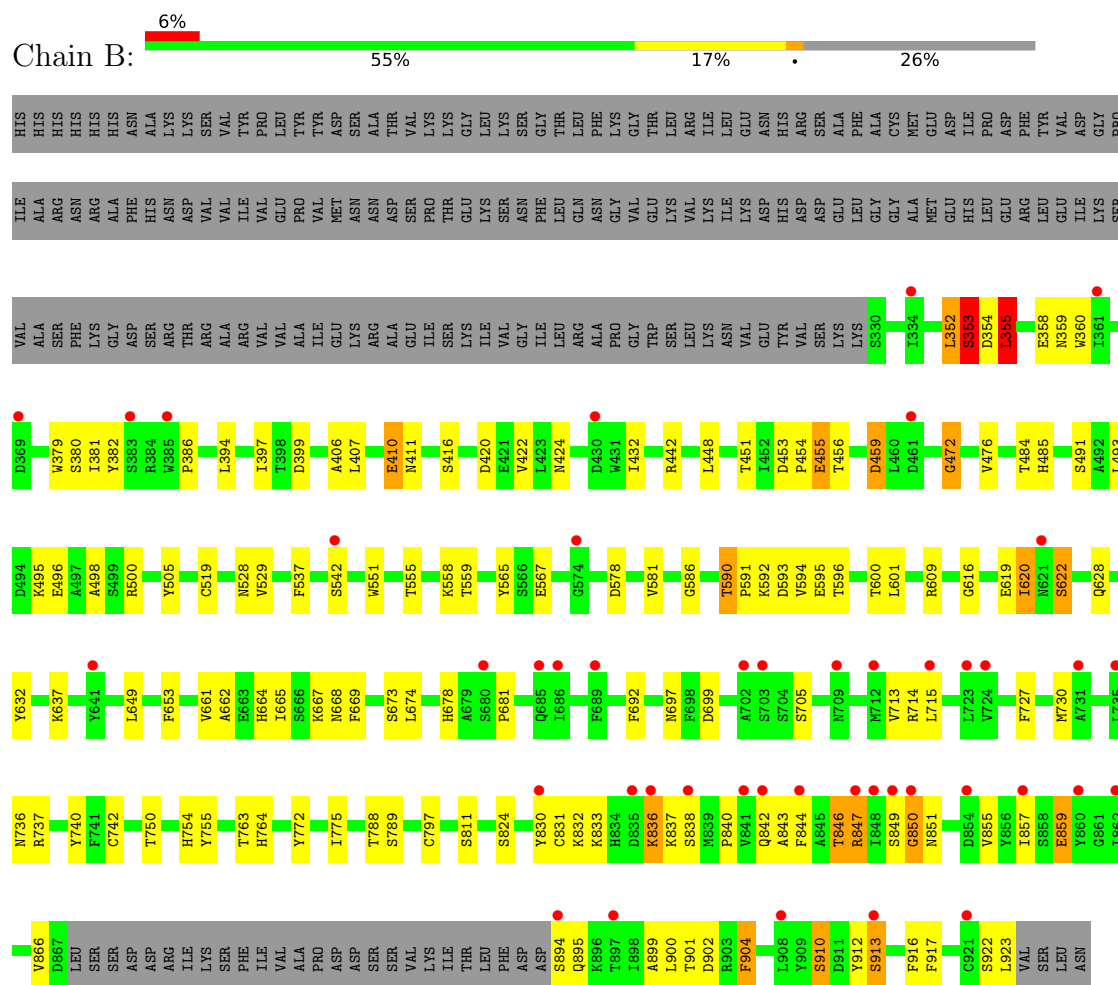
There are 12 discrepancies between the modelled and reference sequences:

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

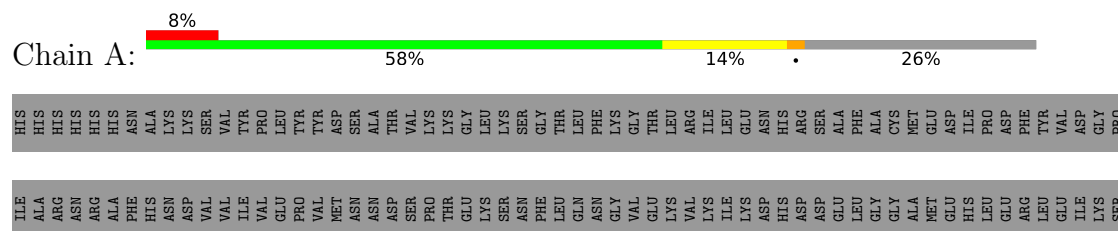
3 Residue-property plots

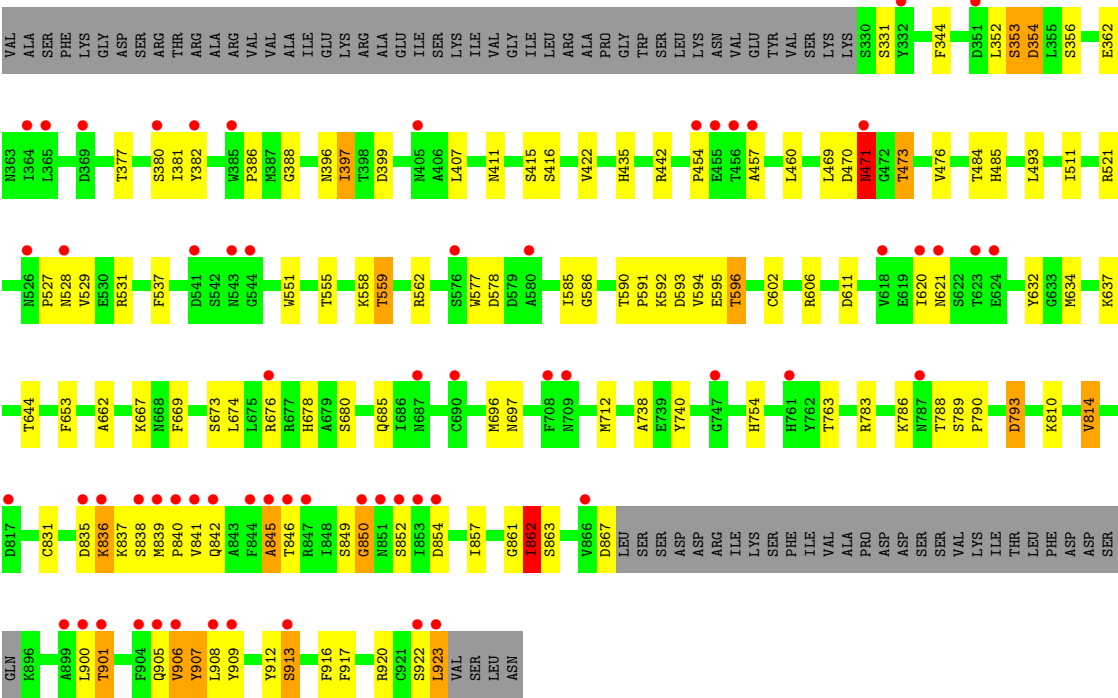
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: DIS3-like exonuclease 2





4 Data and refinement statistics

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 40.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.53-2.80) 99.4 (40.53-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.269 , 0.294 0.289 , 0.300	Depositor DCC
R_{free} test set	1890 reflections (4.96%)	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 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	1/4174 (0.0%)	0.97	21/5700 (0.4%)
1	B	0.46	3/4284 (0.1%)	0.97	21/5840 (0.4%)
All	All	0.46	4/8458 (0.0%)	0.97	42/11540 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	ALA	N-CA	-6.20	1.38	1.46
1	B	359	ASN	N-CA	5.78	1.55	1.46
1	B	352	LEU	C-N	-5.74	1.25	1.33
1	B	358	GLU	CA-C	-5.19	1.46	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	908	LEU	N-CA-C	11.46	124.32	110.91
1	B	355	LEU	N-CA-C	-10.39	101.36	114.56
1	A	837	LYS	N-CA-C	10.30	126.70	110.32
1	A	907	TYR	N-CA-C	9.16	124.45	112.72
1	B	837	LYS	N-CA-C	8.50	122.75	109.07
1	A	850	GLY	N-CA-C	8.31	121.08	111.36
1	B	622	SER	N-CA-C	7.75	121.21	110.35
1	A	863	SER	N-CA-C	7.63	121.30	110.23
1	A	471	ASN	N-CA-C	-6.96	99.07	109.86
1	A	621	ASN	N-CA-CB	-6.66	100.51	110.90
1	B	836	LYS	CB-CA-C	-6.59	107.11	116.34
1	B	697	ASN	N-CA-C	6.36	119.87	111.28
1	B	859	GLU	N-CA-C	-6.32	100.96	110.24
1	A	697	ASN	N-CA-C	6.30	120.57	111.56
1	A	685	GLN	CB-CA-C	-6.23	101.00	111.02
1	B	832	LYS	N-CA-C	-6.16	105.81	113.38
1	B	830	TYR	N-CA-C	-6.14	105.81	113.55
1	B	847	ARG	N-CA-CB	-5.92	100.44	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	846	THR	N-CA-C	5.89	121.43	112.54
1	A	836	LYS	N-CA-C	-5.88	98.27	110.80
1	A	845	ALA	N-CA-C	5.85	117.93	108.34
1	A	901	THR	N-CA-CB	-5.80	108.30	114.10
1	B	455	GLU	CB-CA-C	-5.77	99.33	110.35
1	A	454	PRO	CB-CA-C	-5.76	102.75	111.44
1	A	485	HIS	N-CA-C	-5.75	106.43	113.50
1	B	837	LYS	N-CA-CB	-5.74	101.56	110.57
1	A	470	ASP	N-CA-C	5.70	119.33	112.38
1	B	352	LEU	CA-C-N	5.64	132.31	121.54
1	B	352	LEU	C-N-CA	5.64	132.31	121.54
1	B	472	GLY	N-CA-C	-5.51	100.11	113.18
1	B	485	HIS	N-CA-C	-5.45	106.80	113.50
1	A	849	SER	N-CA-C	5.40	122.31	110.80
1	A	470	ASP	CB-CA-C	-5.37	99.00	110.32
1	A	839	MET	CA-C-N	5.35	126.53	119.84
1	A	839	MET	C-N-CA	5.35	126.53	119.84
1	A	862	ILE	N-CA-C	5.34	120.45	109.34
1	A	331	SER	N-CA-C	-5.29	106.05	112.88
1	B	456	THR	N-CA-CB	5.18	119.25	110.49
1	B	620	ILE	N-CA-CB	-5.17	102.71	111.23
1	B	619	GLU	N-CA-C	5.14	117.04	107.99
1	B	353	SER	N-CA-CB	5.02	118.98	110.49
1	B	833	LYS	CB-CA-C	5.01	119.74	109.67

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	60	0
1	B	4193	0	3765	79	0
All	All	8275	0	7335	139	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 (139) 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: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:353:SER:O	1:B:354:ASP:CG	2.45	0.60
1:B:831:CYS:HB3	1:B:836:LYS:O	2.01	0.60
1:A:669:PHE:O	1:A:673:SER:OG	2.20	0.59
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
1:A:841:VAL:HA	1:A:905:GLN:HA	1.86	0.58
1:B:727:PHE:HA	1:B:730:MET:HE2	1.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:380:SER:C	1:B:382:TYR:H	2.21	0.47
1:B:692:PHE:CE1	1:B:730:MET:HE1	2.49	0.47
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:PHE:CD1	1:A:790:PRO:HG3	2.50	0.47
1:A:835:ASP:O	1:A:836:LYS:C	2.58	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:380:SER:C	1:A:382:TYR:H	2.23	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:360:TRP:H	1:B:360:TRP:CD1	2.33	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:B:596:THR:O	1:B:600:THR:OG1	2.30	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:669:PHE:O	1:B:673:SER:OG	2.33	0.44
1:B:850:GLY:CA	1:B:851:ASN:CB	2.96	0.44
1:A:396:ASN:HB3	1:A:634:MET:HE2	2.00	0.44
1:B:899:ALA:O	1:B:900:LEU:C	2.60	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: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: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
1:A:906:VAL:HB	1:A:907:TYR:H	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	55
1	B	564/764 (74%)	487 (86%)	73 (13%)	4 (1%)	18	47
All	All	1126/1528 (74%)	981 (87%)	138 (12%)	7 (1%)	21	51

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%)	345 (92%)	28 (8%)	12	37
1	B	406/683 (59%)	383 (94%)	23 (6%)	18	49
All	All	779/1366 (57%)	728 (94%)	51 (6%)	15	43

All (51) 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	432	ILE
1	B	459	ASP
1	B	519	CYS
1	B	529	VAL
1	B	542	SER
1	B	558	LYS
1	B	578	ASP
1	B	590	THR
1	B	609	ARG
1	B	622	SER
1	B	668	ASN
1	B	713	VAL
1	B	715	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	397	ILE
1	A	416	SER
1	A	435	HIS
1	A	471	ASN
1	A	473	THR
1	A	484	THR
1	A	529	VAL
1	A	558	LYS
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	667	LYS
1	A	680	SER
1	A	696	MET
1	A	712	MET
1	A	786	LYS
1	A	793	ASP
1	A	814	VAL
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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	671	ASN
1	A	367	HIS
1	A	435	HIS
1	A	664	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.94	63 (11%) 10 7	41, 66, 94, 109	0
1	B	568/764 (74%)	0.67	44 (7%) 19 14	28, 50, 91, 103	0
All	All	1134/1528 (74%)	0.81	107 (9%) 14 10	28, 59, 93, 109	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	921	CYS	5.7
1	A	623	THR	5.2
1	A	908	LEU	4.9
1	A	385	TRP	4.8
1	B	894	SER	4.5
1	A	838	SER	4.4
1	A	842	GLN	3.8
1	B	838	SER	3.7
1	A	787	ASN	3.7
1	A	845	ALA	3.7
1	B	723	LEU	3.6
1	B	836	LYS	3.5
1	A	836	LYS	3.5
1	B	703	SER	3.5
1	B	641	TYR	3.5
1	A	841	VAL	3.5
1	B	913	SER	3.4
1	B	686	ILE	3.4
1	A	846	THR	3.3
1	B	542	SER	3.3
1	B	702	ALA	3.2
1	B	383	SER	3.1
1	A	621	ASN	3.1
1	A	850	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	923	LEU	2.9
1	B	850	GLY	2.9
1	B	369	ASP	2.9
1	B	847	ARG	2.9
1	B	680	SER	2.9
1	A	380	SER	2.9
1	B	709	ASN	2.8
1	B	735	LEU	2.8
1	B	724	VAL	2.8
1	B	848	ILE	2.8
1	A	620	ILE	2.8
1	A	543	ASN	2.8
1	B	621	ASN	2.7
1	A	687	ASN	2.7
1	B	842	GLN	2.7
1	A	817	ASP	2.7
1	A	900	LEU	2.7
1	A	382	TYR	2.7
1	A	576	SER	2.7
1	B	689	PHE	2.6
1	A	456	THR	2.6
1	A	364	ILE	2.6
1	A	840	PRO	2.6
1	A	901	THR	2.6
1	A	405	ASN	2.6
1	A	369	ASP	2.6
1	A	851	ASN	2.6
1	A	332	TYR	2.5
1	B	685	GLN	2.5
1	B	862	ILE	2.5
1	A	847	ARG	2.5
1	A	906	VAL	2.5
1	B	835	ASP	2.4
1	A	854	ASP	2.4
1	A	708	PHE	2.4
1	A	909	TYR	2.4
1	A	835	ASP	2.4
1	A	624	GLU	2.4
1	B	849	SER	2.4
1	A	618	VAL	2.4
1	A	844	PHE	2.4
1	B	334	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	841	VAL	2.3
1	B	731	ALA	2.3
1	A	471	ASN	2.3
1	A	580	ALA	2.3
1	B	430	ASP	2.3
1	A	913	SER	2.3
1	B	574	GLY	2.3
1	B	715	LEU	2.3
1	A	676	ARG	2.2
1	A	526	ASN	2.2
1	B	854	ASP	2.2
1	A	866	VAL	2.2
1	B	830	TYR	2.2
1	B	860	TYR	2.2
1	B	844	PHE	2.2
1	A	541	ASP	2.2
1	B	908	LEU	2.2
1	A	455	GLU	2.2
1	B	361	ILE	2.1
1	A	528	ASN	2.1
1	A	454	PRO	2.1
1	B	461	ASP	2.1
1	B	712	MET	2.1
1	A	544	GLY	2.1
1	A	365	LEU	2.1
1	A	853	ILE	2.1
1	A	899	ALA	2.1
1	B	897	THR	2.1
1	A	457	ALA	2.1
1	A	690	CYS	2.1
1	A	922	SER	2.1
1	A	747	GLY	2.1
1	A	351	ASP	2.1
1	B	857	ILE	2.1
1	A	852	SER	2.0
1	A	761	HIS	2.0
1	A	905	GLN	2.0
1	A	709	ASN	2.0
1	B	385	TRP	2.0
1	A	904	PHE	2.0
1	A	839	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.