



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:04 PM UTC

PDB ID : 1WLH / pdb_00001wlh
Title : Molecular structure of the rod domain of Dictyostelium filamin
Authors : Popowicz, G.M.; Mueller, R.; Noegel, A.A.; Schleicher, M.; Huber, R.; Holak, T.A.
Deposited on : 2004-06-27
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

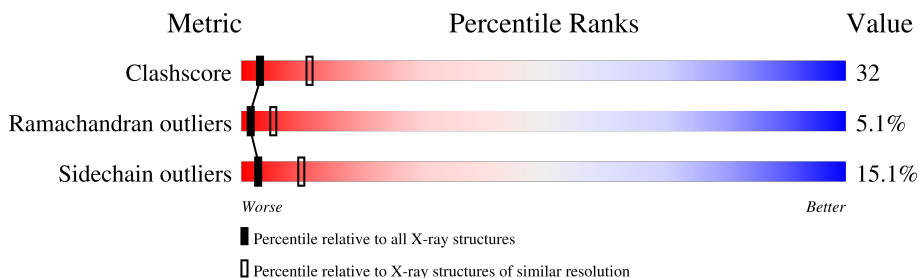
1 Overall quality at a glance

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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4625 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 Gelation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2275	1424	371	476	4			
1	B	306	Total	C	N	O	S	0	0	0
			2262	1417	369	472	4			

- Molecule 2 is water.

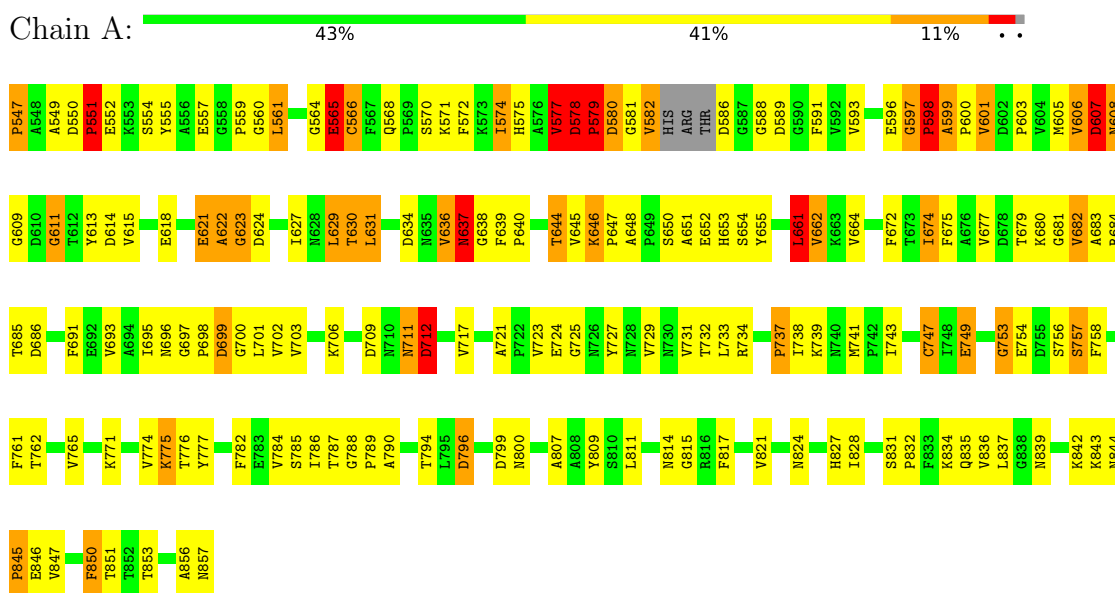
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	53	Total	O	0	0
			53	53		

3 Residue-property plots

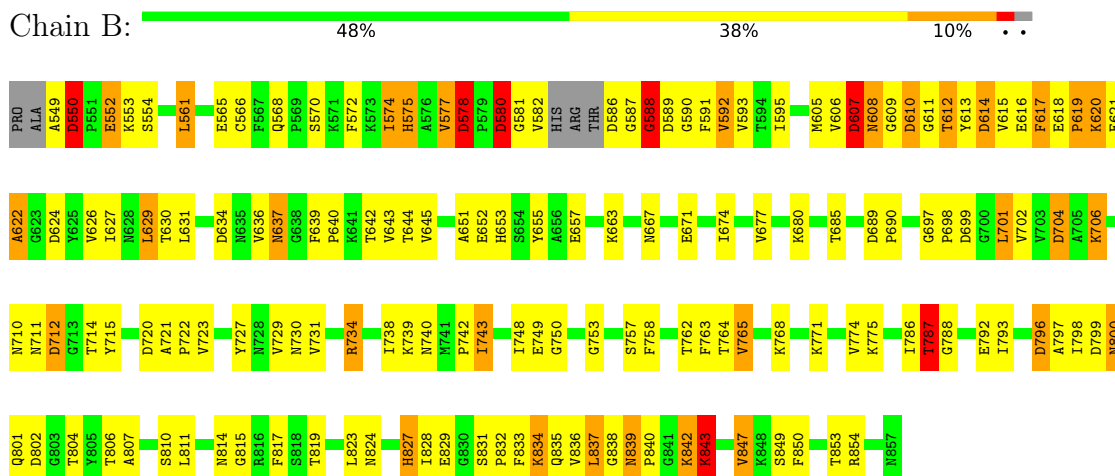
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Gelation factor



- Molecule 1: Gelation factor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.32Å 61.67Å 119.03Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.0 (30.00-2.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.257 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4625	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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	1.05	7/2324 (0.3%)	1.70	44/3161 (1.4%)
1	B	0.94	3/2310 (0.1%)	1.53	35/3141 (1.1%)
All	All	1.00	10/4634 (0.2%)	1.62	79/6302 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	12
1	B	0	7
All	All	1	19

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	618	GLU	C-N	8.80	1.43	1.33
1	A	550	ASP	C-N	7.88	1.43	1.34
1	A	598	PRO	C-O	-7.20	1.14	1.24
1	A	578	ASP	N-CA	5.83	1.54	1.46
1	A	608	ASN	C-O	-5.39	1.17	1.23
1	A	578	ASP	C-N	5.08	1.45	1.33
1	B	575	HIS	CG-ND1	-5.07	1.32	1.38
1	A	827	HIS	CG-ND1	-5.07	1.32	1.38
1	A	575	HIS	CG-ND1	-5.03	1.32	1.38
1	B	827	HIS	CG-ND1	-5.02	1.32	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	ASP	CA-C-N	-13.74	102.67	119.84
1	A	578	ASP	C-N-CA	-13.74	102.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	ASP	CA-CB-CG	12.81	125.41	112.60
1	B	618	GLU	CA-C-N	-11.83	106.76	120.13
1	B	618	GLU	C-N-CA	-11.83	106.76	120.13
1	B	578	ASP	CA-C-N	11.66	134.41	119.84
1	B	578	ASP	C-N-CA	11.66	134.41	119.84
1	A	550	ASP	CA-C-N	-11.51	106.30	118.85
1	A	550	ASP	C-N-CA	-11.51	106.30	118.85
1	A	646	LYS	CA-C-N	-9.77	110.52	120.98
1	A	646	LYS	C-N-CA	-9.77	110.52	120.98
1	A	712	ASP	CA-CB-CG	9.56	122.16	112.60
1	A	566	CYS	N-CA-C	8.88	122.07	111.33
1	A	824	ASN	O-C-N	-8.77	112.05	122.58
1	A	599	ALA	CA-C-N	-8.74	111.42	120.85
1	A	599	ALA	C-N-CA	-8.74	111.42	120.85
1	A	608	ASN	CA-CB-CG	8.46	121.06	112.60
1	B	622	ALA	N-CA-C	8.33	123.16	109.24
1	A	824	ASN	CA-C-O	8.13	131.17	121.65
1	B	617	PHE	O-C-N	-8.12	111.79	122.59
1	B	589	ASP	CA-CB-CG	8.10	120.70	112.60
1	B	704	ASP	CA-CB-CG	8.02	120.62	112.60
1	B	580	ASP	CA-CB-CG	7.98	120.58	112.60
1	B	550	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	579	PRO	CA-C-N	7.48	135.38	122.81
1	A	579	PRO	C-N-CA	7.48	135.38	122.81
1	A	551	PRO	CA-N-CD	-7.21	101.91	112.00
1	A	561	LEU	CB-CA-C	7.14	122.73	110.94
1	B	607	ASP	CA-C-N	6.91	134.42	122.81
1	B	607	ASP	C-N-CA	6.91	134.42	122.81
1	A	578	ASP	N-CA-C	-6.86	94.66	109.81
1	A	561	LEU	N-CA-CB	-6.85	100.49	110.70
1	B	697	GLY	CA-C-N	-6.84	111.28	119.84
1	B	697	GLY	C-N-CA	-6.84	111.28	119.84
1	B	802	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	618	GLU	CA-C-O	6.71	126.43	120.19
1	B	619	PRO	CA-N-CD	-6.54	102.84	112.00
1	A	550	ASP	C-N-CD	6.53	151.79	125.00
1	B	622	ALA	O-C-N	6.23	130.87	123.27
1	B	618	GLU	C-N-CD	6.17	150.30	125.00
1	A	565	GLU	CA-C-N	6.17	128.83	120.38
1	A	565	GLU	C-N-CA	6.17	128.83	120.38
1	A	550	ASP	CA-C-O	6.16	127.14	120.05
1	A	799	ASP	CA-CB-CG	6.16	118.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	GLY	CA-C-N	6.14	134.38	121.91
1	B	588	GLY	C-N-CA	6.14	134.38	121.91
1	B	589	ASP	O-C-N	-6.13	117.39	123.46
1	B	712	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	607	ASP	N-CA-C	6.07	120.45	112.13
1	A	589	ASP	N-CA-CB	-6.05	102.30	111.19
1	A	734	ARG	CA-C-O	6.03	128.45	121.28
1	B	561	LEU	N-CA-CB	-5.95	101.83	110.70
1	A	637	ASN	CA-CB-CG	5.95	118.55	112.60
1	B	581	GLY	O-C-N	5.95	130.43	122.70
1	B	618	GLU	N-CA-C	-5.93	102.13	110.31
1	A	661	LEU	CA-C-O	5.79	126.34	119.56
1	B	605	MET	CA-CB-CG	-5.79	102.52	114.10
1	B	608	ASN	N-CA-C	5.72	118.88	109.85
1	B	698	PRO	N-CA-CB	5.68	109.22	103.25
1	B	578	ASP	N-CA-C	5.66	122.33	109.81
1	A	581	GLY	N-CA-C	5.66	116.88	111.67
1	A	579	PRO	O-C-N	5.65	130.26	122.64
1	A	549	ALA	N-CA-C	5.64	117.81	110.53
1	A	577	VAL	CG1-CB-CG2	-5.61	98.46	110.80
1	A	549	ALA	O-C-N	-5.53	115.85	122.65
1	A	646	LYS	O-C-N	5.41	127.75	121.21
1	A	580	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	699	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	577	VAL	N-CA-CB	-5.33	105.06	112.52
1	B	787	THR	CA-CB-CG2	5.31	119.52	110.50
1	A	597	GLY	CA-C-N	5.29	126.45	119.84
1	A	597	GLY	C-N-CA	5.29	126.45	119.84
1	A	662	VAL	N-CA-C	-5.24	106.56	111.48
1	A	566	CYS	O-C-N	-5.23	116.58	122.12
1	A	661	LEU	O-C-N	-5.18	116.12	122.34
1	B	614	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	698	PRO	CA-C-N	-5.03	114.59	122.95
1	B	698	PRO	C-N-CA	-5.03	114.59	122.95
1	A	622	ALA	O-C-N	5.02	127.98	123.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	548	ALA	CA

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	547	PRO	Mainchain
1	A	551	PRO	Mainchain
1	A	565	GLU	Mainchain
1	A	578	ASP	Mainchain,Peptide
1	A	606	VAL	Mainchain,Peptide
1	A	609	GLY	Peptide
1	A	644	THR	Mainchain
1	A	662	VAL	Mainchain
1	A	712	ASP	Sidechain
1	A	842	LYS	Mainchain
1	B	578	ASP	Peptide
1	B	607	ASP	Mainchain
1	B	612	THR	Mainchain
1	B	617	PHE	Mainchain
1	B	685	THR	Mainchain
1	B	711	ASN	Mainchain
1	B	734	ARG	Mainchain

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	2275	0	2151	176	1
1	B	2262	0	2140	119	2
2	A	35	0	0	21	0
2	B	53	0	0	14	0
All	All	4625	0	4291	279	2

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 32.

All (279) 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:579:PRO:CG	2:A:14:HOH:O	1.82	1.25
1:A:605:MET:HE3	1:A:607:ASP:OD1	1.31	1.25
1:A:681:GLY:HA2	2:A:59:HOH:O	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:GLY:O	1:B:588:GLY:O	1.65	1.15
1:A:654:SER:HB2	2:A:87:HOH:O	1.48	1.12
1:A:547:PRO:HD3	2:A:10:HOH:O	1.52	1.08
1:B:723:VAL:HG23	2:B:86:HOH:O	1.52	1.08
1:A:598:PRO:HG2	1:A:622:ALA:HB1	1.31	1.07
1:B:701:LEU:HA	2:B:79:HOH:O	1.54	1.05
1:B:582:VAL:HG21	2:B:35:HOH:O	1.55	1.05
1:A:607:ASP:HB3	1:A:608:ASN:OD1	1.55	1.05
1:A:579:PRO:HG2	2:A:14:HOH:O	1.51	1.00
1:B:587:GLY:O	1:B:588:GLY:C	2.05	0.99
1:B:608:ASN:HB3	1:B:612:THR:O	1.62	0.99
1:A:685:THR:C	1:A:712:ASP:O	2.06	0.98
1:A:685:THR:HG22	2:A:53:HOH:O	1.65	0.97
1:B:614:ASP:OD2	2:B:33:HOH:O	1.82	0.96
1:B:630:THR:HB	1:B:634:ASP:H	1.33	0.94
1:A:738:ILE:HB	2:A:87:HOH:O	1.67	0.94
1:A:652:GLU:HB2	2:A:78:HOH:O	1.68	0.93
1:A:815:GLY:HA3	2:A:84:HOH:O	1.67	0.93
1:A:857:ASN:HA	2:A:1:HOH:O	1.67	0.93
1:A:566:CYS:SG	1:A:647:PRO:HA	2.12	0.90
1:A:844:ASN:OD1	1:A:845:PRO:HD2	1.72	0.89
1:B:796:ASP:OD2	1:B:798:ILE:HD11	1.72	0.89
1:A:685:THR:O	1:A:712:ASP:O	1.91	0.89
1:A:570:SER:HA	2:A:85:HOH:O	1.73	0.87
1:A:789:PRO:CB	1:A:843:LYS:NZ	2.39	0.86
1:B:565:GLU:OE2	1:B:568:GLN:HG3	1.77	0.84
1:B:706:LYS:HD2	2:B:60:HOH:O	1.77	0.83
1:B:587:GLY:C	1:B:588:GLY:O	2.21	0.82
1:B:814:ASN:HB3	1:B:843:LYS:HB3	1.60	0.82
1:A:650:SER:HB2	1:A:653:HIS:HB2	1.62	0.82
1:A:607:ASP:O	1:A:613:TYR:HA	1.80	0.81
2:A:19:HOH:O	1:B:764:THR:HG23	1.81	0.80
1:A:605:MET:CE	1:A:607:ASP:OD1	2.24	0.80
1:B:608:ASN:CB	1:B:612:THR:O	2.30	0.79
1:A:607:ASP:OD1	1:A:613:TYR:HD2	1.65	0.79
1:A:650:SER:OG	1:A:679:THR:HA	1.84	0.77
1:A:789:PRO:HG2	2:A:84:HOH:O	1.83	0.76
1:B:550:ASP:OD2	1:B:578:ASP:HA	1.86	0.76
1:A:731:VAL:O	1:A:738:ILE:HG12	1.85	0.75
1:A:605:MET:HE3	1:A:607:ASP:CG	2.11	0.75
1:B:722:PRO:HB2	2:B:86:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LEU:HD13	1:A:741:MET:HE1	1.69	0.75
1:A:566:CYS:SG	1:A:621:GLU:CD	2.70	0.74
1:A:639:PHE:HB3	1:A:640:PRO:HA	1.70	0.74
1:A:655:TYR:HB3	1:A:739:LYS:HG2	1.70	0.73
1:A:828:ILE:HD11	1:B:758:PHE:CZ	2.24	0.73
1:A:685:THR:O	1:A:712:ASP:HA	1.89	0.73
1:A:607:ASP:OD1	1:A:613:TYR:CD2	2.42	0.72
1:A:695:ILE:HG22	1:A:703:VAL:HB	1.72	0.71
1:A:789:PRO:CB	1:A:843:LYS:HZ1	2.04	0.70
1:A:789:PRO:CG	1:A:843:LYS:HZ3	2.03	0.70
1:A:789:PRO:HB3	1:A:843:LYS:HZ1	1.56	0.70
1:B:566:CYS:SG	1:B:622:ALA:HB2	2.32	0.70
1:A:560:GLY:HA2	2:A:27:HOH:O	1.93	0.69
1:A:564:GLY:O	1:A:646:LYS:HG2	1.93	0.68
1:B:624:ASP:OD2	1:B:644:THR:HG22	1.94	0.68
1:A:723:VAL:HG12	1:A:724:GLU:O	1.93	0.68
1:A:698:PRO:HD3	1:A:727:TYR:CZ	2.28	0.68
1:A:551:PRO:HA	1:A:631:LEU:HD22	1.77	0.67
1:A:695:ILE:HG13	1:A:729:VAL:HG22	1.76	0.66
1:A:674:ILE:HD11	1:A:717:VAL:HG21	1.77	0.66
1:A:697:GLY:HA2	1:A:727:TYR:HA	1.75	0.66
1:A:775:LYS:HG2	1:B:749:GLU:OE1	1.94	0.66
1:A:789:PRO:CB	1:A:843:LYS:HZ3	2.07	0.66
1:A:789:PRO:HB2	1:A:843:LYS:NZ	2.09	0.66
1:B:722:PRO:C	2:B:86:HOH:O	2.38	0.66
1:A:574:ILE:HD13	1:A:629:LEU:HD11	1.76	0.66
1:B:606:VAL:HG13	1:B:614:ASP:HB2	1.77	0.66
1:A:695:ILE:CG2	1:A:703:VAL:HB	2.26	0.66
1:B:574:ILE:HB	1:B:613:TYR:HB2	1.77	0.65
1:B:651:ALA:O	1:B:738:ILE:HA	1.96	0.65
1:B:582:VAL:HG12	2:B:17:HOH:O	1.97	0.65
1:A:579:PRO:CD	2:A:14:HOH:O	2.24	0.64
1:B:854:ARG:HH11	1:B:854:ARG:HG2	1.62	0.64
1:A:664:VAL:O	1:A:747:CYS:HA	1.98	0.64
1:A:789:PRO:HG2	1:A:843:LYS:HZ3	1.61	0.64
1:A:782:PHE:HB3	1:A:856:ALA:HB3	1.80	0.64
1:B:606:VAL:CG1	1:B:614:ASP:HB2	2.28	0.64
1:A:796:ASP:O	1:A:807:ALA:HA	1.98	0.64
1:A:623:GLY:HA2	1:A:645:VAL:O	1.99	0.63
1:A:685:THR:O	1:A:712:ASP:C	2.41	0.63
1:B:836:VAL:O	1:B:837:LEU:HD13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:PRO:HB3	2:A:49:HOH:O	1.99	0.62
1:A:709:ASP:OD1	1:A:711:ASN:OD1	2.18	0.62
1:A:554:SER:HA	1:A:577:VAL:HG23	1.79	0.62
1:B:630:THR:HB	1:B:634:ASP:N	2.10	0.61
1:A:845:PRO:HA	2:A:88:HOH:O	2.00	0.61
1:B:582:VAL:CG1	2:B:17:HOH:O	2.47	0.61
1:A:757:SER:C	1:B:765:VAL:HG12	2.25	0.60
1:B:764:THR:HG22	1:B:806:THR:HG23	1.83	0.60
1:A:814:ASN:HB3	1:A:839:ASN:O	2.00	0.60
1:A:629:LEU:O	1:A:636:VAL:HG23	2.01	0.60
1:A:655:TYR:HA	1:A:739:LYS:HB3	1.82	0.60
1:B:722:PRO:CB	2:B:86:HOH:O	2.44	0.60
1:A:775:LYS:HE3	1:B:749:GLU:O	2.02	0.60
1:A:756:SER:O	1:B:829:GLU:HG3	2.02	0.59
1:A:566:CYS:SG	1:A:621:GLU:OE2	2.60	0.59
1:B:608:ASN:HD22	1:B:610:ASP:C	2.08	0.59
1:A:653:HIS:CD2	2:A:59:HOH:O	2.55	0.58
1:A:850:PHE:HD1	1:A:850:PHE:H	1.49	0.58
1:B:565:GLU:OE2	1:B:734:ARG:NH2	2.35	0.58
1:A:655:TYR:CE2	1:A:675:PHE:CD1	2.91	0.58
1:A:661:LEU:HD21	1:A:672:PHE:CE2	2.39	0.58
1:A:685:THR:O	1:A:712:ASP:CA	2.52	0.58
1:B:552:GLU:HA	1:B:637:ASN:HB2	1.86	0.57
1:A:775:LYS:HD2	1:A:777:TYR:O	2.04	0.57
1:A:568:GLN:C	1:A:618:GLU:HG3	2.30	0.57
1:A:598:PRO:HG2	1:A:622:ALA:CB	2.22	0.57
1:A:677:VAL:HG13	1:A:682:VAL:O	2.05	0.57
1:A:572:PHE:CZ	1:A:615:VAL:HG11	2.41	0.56
1:B:608:ASN:ND2	1:B:610:ASP:O	2.22	0.56
1:A:564:GLY:HA3	1:A:645:VAL:HG22	1.87	0.56
1:A:661:LEU:HD13	1:A:741:MET:CE	2.35	0.56
1:A:757:SER:O	1:B:765:VAL:HG12	2.05	0.56
1:A:758:PHE:HE1	1:B:763:PHE:CD1	2.23	0.56
1:A:788:GLY:HA3	1:A:817:PHE:CE1	2.40	0.56
1:A:789:PRO:CG	1:A:843:LYS:NZ	2.67	0.56
1:A:566:CYS:SG	1:A:621:GLU:HA	2.46	0.56
1:B:671:GLU:HB3	2:B:11:HOH:O	2.05	0.56
1:A:559:PRO:O	1:A:571:LYS:O	2.24	0.55
1:A:693:VAL:HG13	1:A:731:VAL:HG22	1.87	0.55
1:A:850:PHE:HD1	1:A:850:PHE:N	2.04	0.55
1:B:595:ILE:HG13	1:B:627:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:PHE:HE1	1:A:674:ILE:CD1	2.19	0.55
1:A:693:VAL:HG12	1:A:695:ILE:CD1	2.36	0.55
1:A:753:GLY:HA2	1:B:823:LEU:HB2	1.89	0.55
1:B:565:GLU:O	1:B:619:PRO:HG2	2.06	0.55
1:A:790:ALA:HB3	1:A:850:PHE:CZ	2.42	0.55
1:A:709:ASP:OD1	1:A:711:ASN:CG	2.50	0.55
1:A:794:THR:O	1:A:809:TYR:HA	2.07	0.55
1:B:549:ALA:HA	1:B:577:VAL:O	2.07	0.54
1:B:814:ASN:CB	1:B:843:LYS:HB3	2.35	0.54
1:A:574:ILE:HB	1:A:613:TYR:HB2	1.90	0.54
1:A:828:ILE:HD11	1:B:758:PHE:CE1	2.42	0.54
1:A:850:PHE:N	1:A:850:PHE:CD1	2.75	0.54
1:B:606:VAL:C	1:B:607:ASP:O	2.49	0.54
1:A:579:PRO:HG3	2:A:14:HOH:O	1.77	0.54
1:A:565:GLU:N	1:A:645:VAL:HG13	2.22	0.54
1:A:753:GLY:O	1:A:756:SER:HB2	2.08	0.54
1:B:799:ASP:C	1:B:801:GLN:H	2.15	0.54
1:A:577:VAL:HG12	1:A:580:ASP:C	2.33	0.53
1:A:651:ALA:O	1:A:738:ILE:HA	2.08	0.53
1:A:608:ASN:HB3	1:A:613:TYR:CE2	2.44	0.53
1:A:835:GLN:HA	1:B:834:LYS:O	2.08	0.53
1:B:577:VAL:HG13	1:B:580:ASP:N	2.22	0.53
1:A:698:PRO:HG3	1:A:725:GLY:HA3	1.90	0.53
1:B:788:GLY:HA3	1:B:817:PHE:CE2	2.43	0.52
1:B:554:SER:HB2	1:B:575:HIS:O	2.10	0.52
1:A:749:GLU:HB3	1:B:775:LYS:HE3	1.91	0.52
1:A:650:SER:HG	1:A:679:THR:HA	1.74	0.52
1:A:674:ILE:N	1:A:674:ILE:HD13	2.25	0.52
1:B:565:GLU:CD	1:B:568:GLN:HG3	2.35	0.52
1:A:738:ILE:O	1:A:741:MET:HB2	2.10	0.51
1:B:591:PHE:CE2	1:B:613:TYR:CE1	2.98	0.51
1:B:608:ASN:CG	1:B:612:THR:O	2.54	0.51
1:B:819:THR:HB	1:B:833:PHE:CE1	2.44	0.51
1:A:682:VAL:HG12	1:A:683:ALA:H	1.75	0.51
1:A:566:CYS:HG	1:A:647:PRO:HA	1.76	0.51
1:A:577:VAL:HG12	1:A:580:ASP:CA	2.41	0.51
1:B:655:TYR:N	1:B:655:TYR:CD1	2.79	0.50
1:A:774:VAL:HG12	1:A:775:LYS:O	2.12	0.50
1:A:597:GLY:C	1:A:599:ALA:H	2.19	0.50
1:B:565:GLU:O	1:B:645:VAL:HG13	2.12	0.50
1:B:701:LEU:HD12	1:B:702:VAL:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:ALA:HB1	1:B:727:TYR:CE1	2.47	0.50
1:A:737:PRO:HB2	1:A:741:MET:O	2.12	0.49
1:A:639:PHE:HB3	1:A:640:PRO:CA	2.41	0.49
1:A:691:PHE:CE1	1:A:733:LEU:HD13	2.48	0.49
1:B:762:THR:HA	1:B:807:ALA:O	2.12	0.49
1:A:566:CYS:HB2	1:A:648:ALA:HB2	1.93	0.49
1:B:639:PHE:HA	1:B:640:PRO:C	2.38	0.49
1:A:784:VAL:HG21	1:A:807:ALA:HB2	1.95	0.48
1:A:789:PRO:HB2	1:A:843:LYS:HZ3	1.76	0.48
1:A:554:SER:HB2	1:A:577:VAL:N	2.29	0.48
1:A:672:PHE:CE1	1:A:674:ILE:CD1	2.96	0.48
1:B:619:PRO:HG3	1:B:645:VAL:CG2	2.44	0.48
1:B:796:ASP:O	1:B:807:ALA:HA	2.14	0.48
1:B:572:PHE:CE2	1:B:615:VAL:HG11	2.48	0.48
1:A:582:VAL:HG21	1:A:586:ASP:OD2	2.14	0.48
1:A:721:ALA:HB1	1:A:727:TYR:CZ	2.49	0.48
1:A:661:LEU:CD1	1:A:741:MET:HE1	2.41	0.47
1:A:699:ASP:CG	1:A:699:ASP:O	2.57	0.47
1:B:572:PHE:CE2	1:B:615:VAL:CG1	2.97	0.47
1:B:720:ASP:O	1:B:722:PRO:HD3	2.14	0.47
1:A:672:PHE:CD1	1:A:672:PHE:C	2.92	0.47
1:B:595:ILE:HG13	1:B:627:ILE:HD13	1.96	0.47
1:A:630:THR:HG22	1:A:634:ASP:N	2.29	0.47
1:A:605:MET:CE	1:A:607:ASP:CG	2.83	0.47
1:A:731:VAL:HG12	1:A:738:ILE:HD11	1.96	0.47
1:A:650:SER:CB	1:A:653:HIS:HB2	2.41	0.47
1:A:661:LEU:HD21	1:A:672:PHE:CD2	2.50	0.47
1:A:661:LEU:CD1	1:A:741:MET:CE	2.93	0.47
1:A:686:ASP:HA	1:A:712:ASP:HA	1.96	0.47
1:A:815:GLY:O	1:A:836:VAL:HG13	2.14	0.47
1:A:845:PRO:C	1:A:847:VAL:H	2.22	0.47
1:A:624:ASP:CG	1:A:644:THR:HG22	2.40	0.47
1:B:667:ASN:OD1	1:B:750:GLY:HA3	2.15	0.47
1:A:685:THR:C	1:A:712:ASP:C	2.82	0.46
1:B:710:ASN:HB3	1:B:712:ASP:OD1	2.15	0.46
1:A:732:THR:HG22	1:A:737:PRO:N	2.30	0.46
1:A:831:SER:HA	1:A:832:PRO:C	2.40	0.46
1:A:834:LYS:HG2	1:A:835:GLN:N	2.30	0.46
1:A:674:ILE:HD11	1:A:717:VAL:CG2	2.42	0.46
1:B:570:SER:O	1:B:616:GLU:HA	2.16	0.46
1:B:577:VAL:HG13	1:B:580:ASP:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:HIS:HB3	1:B:831:SER:HB3	1.97	0.46
1:B:721:ALA:HB1	1:B:727:TYR:CZ	2.51	0.46
1:B:739:LYS:HG2	1:B:740:ASN:ND2	2.31	0.46
1:A:828:ILE:HA	1:B:753:GLY:O	2.17	0.45
1:B:582:VAL:HG21	1:B:586:ASP:OD2	2.16	0.45
1:A:572:PHE:CE2	1:A:615:VAL:HG11	2.51	0.45
1:A:591:PHE:HA	1:A:630:THR:O	2.16	0.45
1:A:636:VAL:C	1:A:638:GLY:H	2.23	0.45
1:A:787:THR:HG23	1:A:851:THR:OG1	2.17	0.45
1:B:689:ASP:HB2	1:B:715:TYR:OH	2.17	0.45
1:B:565:GLU:C	1:B:645:VAL:HG13	2.42	0.45
1:B:620:LYS:HB3	2:B:8:HOH:O	2.15	0.45
1:B:639:PHE:HB3	1:B:640:PRO:HA	1.97	0.45
1:B:793:ILE:HA	1:B:810:SER:O	2.16	0.45
1:A:682:VAL:HG12	1:A:683:ALA:N	2.31	0.44
1:B:831:SER:HA	1:B:832:PRO:HA	1.83	0.44
1:A:554:SER:HB2	1:A:577:VAL:H	1.83	0.44
1:A:606:VAL:O	1:A:614:ASP:O	2.35	0.44
1:B:854:ARG:HG2	1:B:854:ARG:NH1	2.27	0.44
1:A:564:GLY:C	1:A:645:VAL:HG13	2.42	0.44
1:A:551:PRO:HG3	1:A:631:LEU:HD23	2.00	0.44
1:B:763:PHE:CD1	1:B:763:PHE:C	2.96	0.44
1:B:577:VAL:CG1	1:B:580:ASP:H	2.31	0.43
1:B:787:THR:HA	1:B:850:PHE:O	2.17	0.43
1:B:582:VAL:CG2	1:B:586:ASP:OD2	2.66	0.43
1:B:729:VAL:HB	1:B:743:ILE:HG23	2.00	0.43
1:B:701:LEU:CA	2:B:79:HOH:O	2.34	0.43
1:A:601:VAL:O	1:A:603:PRO:HD3	2.18	0.43
1:B:714:THR:C	1:B:715:TYR:CD1	2.96	0.43
1:B:574:ILE:HD13	1:B:629:LEU:HD11	2.01	0.43
1:A:731:VAL:CG1	1:A:738:ILE:HD11	2.49	0.43
1:A:790:ALA:HB3	1:A:850:PHE:HZ	1.84	0.43
1:B:797:ALA:C	1:B:798:ILE:HD13	2.44	0.43
1:A:607:ASP:CB	1:A:608:ASN:OD1	2.46	0.42
1:A:621:GLU:OE2	1:A:647:PRO:HB3	2.19	0.42
1:B:674:ILE:HD13	1:B:731:VAL:HG11	2.01	0.42
1:A:560:GLY:CA	2:A:27:HOH:O	2.60	0.42
1:B:710:ASN:C	1:B:712:ASP:H	2.28	0.42
1:A:552:GLU:O	1:A:637:ASN:HB2	2.20	0.42
1:B:591:PHE:CD2	1:B:613:TYR:CZ	3.07	0.42
1:A:577:VAL:HG12	1:A:580:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HD13	1:B:636:VAL:HB	2.02	0.42
1:A:684:ARG:O	1:A:712:ASP:O	2.38	0.42
1:B:722:PRO:HG2	2:B:86:HOH:O	2.20	0.42
1:B:730:ASN:HB2	1:B:742:PRO:HB3	2.01	0.42
1:B:839:ASN:HB3	1:B:842:LYS:HD2	2.02	0.42
1:A:761:PHE:CD2	1:B:763:PHE:HB3	2.55	0.42
1:A:765:VAL:HG13	1:B:757:SER:O	2.20	0.42
1:B:653:HIS:HB3	1:B:677:VAL:HG11	2.01	0.41
1:B:800:ASN:HB2	1:B:804:THR:OG1	2.19	0.41
1:A:762:THR:HA	1:A:807:ALA:O	2.20	0.41
1:A:566:CYS:HB3	1:A:621:GLU:HB2	2.03	0.41
1:A:654:SER:O	1:A:739:LYS:CB	2.69	0.41
1:B:592:VAL:HG13	1:B:630:THR:OG1	2.21	0.41
1:A:630:THR:HG22	1:A:634:ASP:O	2.21	0.41
1:A:684:ARG:HB3	1:A:684:ARG:NH1	2.35	0.41
1:A:698:PRO:HD3	1:A:727:TYR:CE2	2.56	0.41
1:A:800:ASN:O	2:A:20:HOH:O	2.22	0.41
1:A:582:VAL:HG12	1:A:611:GLY:HA3	2.02	0.41
1:B:582:VAL:HB	1:B:586:ASP:OD2	2.21	0.41
1:A:677:VAL:HG13	1:A:681:GLY:O	2.20	0.41
1:B:630:THR:CB	1:B:634:ASP:H	2.17	0.41
1:B:689:ASP:HA	1:B:690:PRO:HD3	1.83	0.41
1:B:710:ASN:HB2	1:B:714:THR:O	2.21	0.41
1:A:758:PHE:CZ	1:B:828:ILE:HD11	2.56	0.40
1:B:815:GLY:HA2	1:B:840:PRO:HG3	2.03	0.40
1:A:555:TYR:H	1:A:555:TYR:HD1	1.66	0.40
1:B:572:PHE:CZ	1:B:615:VAL:HG11	2.56	0.40
1:B:619:PRO:HG3	1:B:645:VAL:HG21	2.04	0.40
1:B:715:TYR:CD1	1:B:715:TYR:N	2.90	0.40
1:A:754:GLU:HA	1:B:827:HIS:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LYS:NZ	1:B:621:GLU:OE2[1_666]	2.10	0.10
1:B:657:GLU:OE2	1:B:699:ASP:OD1[2_445]	2.19	0.01

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	304/311 (98%)	252 (83%)	35 (12%)	17 (6%)	1	4
1	B	302/311 (97%)	256 (85%)	32 (11%)	14 (5%)	2	6
All	All	606/622 (97%)	508 (84%)	67 (11%)	31 (5%)	1	5

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	PRO
1	A	682	VAL
1	B	838	GLY
1	B	843	LYS
1	A	611	GLY
1	A	623	GLY
1	A	700	GLY
1	A	846	GLU
1	B	588	GLY
1	B	607	ASP
1	B	610	ASP
1	B	637	ASN
1	A	601	VAL
1	A	621	GLU
1	A	637	ASN
1	A	845	PRO
1	B	580	ASP
1	B	590	GLY
1	B	800	ASN
1	A	578	ASP
1	A	711	ASN
1	A	588	GLY
1	A	753	GLY
1	B	578	ASP
1	B	824	ASN

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Mol	Chain	Res	Type
1	B	847	VAL
1	A	598	PRO
1	A	737	PRO
1	A	743	ILE
1	B	609	GLY
1	B	611	GLY

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	243/247 (98%)	209 (86%)	34 (14%)	3	12
1	B	241/247 (98%)	202 (84%)	39 (16%)	2	8
All	All	484/494 (98%)	411 (85%)	73 (15%)	3	10

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	GLU
1	A	561	LEU
1	A	574	ILE
1	A	577	VAL
1	A	578	ASP
1	A	582	VAL
1	A	593	VAL
1	A	596	GLU
1	A	607	ASP
1	A	627	ILE
1	A	629	LEU
1	A	630	THR
1	A	631	LEU
1	A	636	VAL
1	A	661	LEU
1	A	674	ILE
1	A	696	ASN

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Mol	Chain	Res	Type
1	A	701	LEU
1	A	702	VAL
1	A	706	LYS
1	A	747	CYS
1	A	749	GLU
1	A	757	SER
1	A	771	LYS
1	A	775	LYS
1	A	776	THR
1	A	785	SER
1	A	786	ILE
1	A	796	ASP
1	A	811	LEU
1	A	821	VAL
1	A	837	LEU
1	A	850	PHE
1	A	853	THR
1	B	550	ASP
1	B	552	GLU
1	B	553	LYS
1	B	561	LEU
1	B	574	ILE
1	B	592	VAL
1	B	593	VAL
1	B	620	LYS
1	B	626	VAL
1	B	629	LEU
1	B	631	LEU
1	B	642	THR
1	B	643	VAL
1	B	652	GLU
1	B	663	LYS
1	B	680	LYS
1	B	701	LEU
1	B	704	ASP
1	B	706	LYS
1	B	743	ILE
1	B	748	ILE
1	B	765	VAL
1	B	768	LYS
1	B	771	LYS
1	B	774	VAL

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Mol	Chain	Res	Type
1	B	786	ILE
1	B	787	THR
1	B	792	GLU
1	B	796	ASP
1	B	811	LEU
1	B	834	LYS
1	B	835	GLN
1	B	837	LEU
1	B	839	ASN
1	B	842	LYS
1	B	843	LYS
1	B	847	VAL
1	B	849	SER
1	B	853	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	827	HIS
1	B	635	ASN
1	B	653	HIS
1	B	730	ASN
1	B	740	ASN
1	B	824	ASN

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 oligosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.