Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID	:	1WLH
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

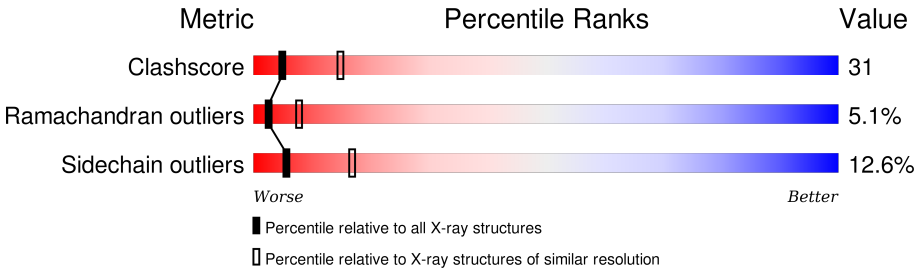
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	311	47% 37% 13%
1	B	311	50% 39% 6%

2 Entry composition (i)

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		

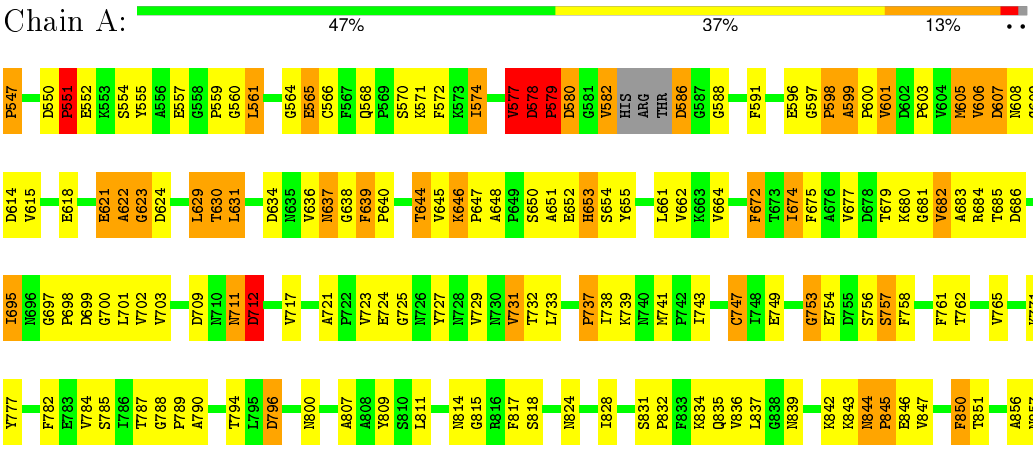
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

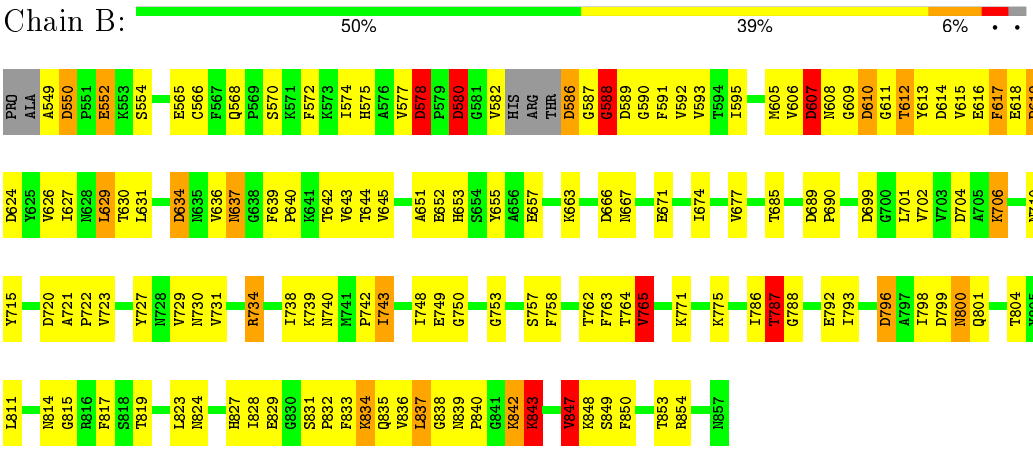
- Molecule 1: Gelation factor

Chain A:



- Molecule 1: Gelation factor

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.75	1/2324 (0.0%)	1.37	23/3161 (0.7%)
1	B	0.69	0/2310	1.28	14/3141 (0.4%)
All	All	0.72	1/4634 (0.0%)	1.33	37/6302 (0.6%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	578	ASP	C-N	6.04	1.45	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	550	ASP	C-N-CD	11.14	151.79	128.40
1	B	618	GLU	C-N-CD	10.43	150.30	128.40
1	A	672	PHE	CB-CG-CD1	-9.19	114.36	120.80
1	B	580	ASP	CB-CG-OD1	8.75	126.18	118.30
1	B	589	ASP	CB-CG-OD2	8.62	126.06	118.30
1	B	586	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	A	577	VAL	CG1-CB-CG2	-7.77	98.46	110.90
1	A	646	LYS	C-N-CD	7.59	144.34	128.40
1	A	712	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	599	ALA	C-N-CD	6.88	142.85	128.40
1	A	551	PRO	CA-N-CD	-6.85	101.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	617	PHE	O-C-N	-6.82	111.79	122.70
1	A	672	PHE	CB-CG-CD2	6.63	125.44	120.80
1	A	561	LEU	CB-CA-C	6.59	122.73	110.20
1	A	824	ASN	O-C-N	-6.56	112.05	123.20
1	A	639	PHE	CB-CG-CD1	-6.53	116.23	120.80
1	A	578	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	605	MET	CA-CB-CG	-6.34	102.52	113.30
1	A	712	ASP	OD1-CG-OD2	-6.29	111.36	123.30
1	B	622	ALA	CA-C-N	-6.20	103.80	116.20
1	B	619	PRO	CA-N-CD	-6.18	102.84	111.50
1	A	586	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	847	VAL	CG1-CB-CG2	-6.05	101.21	110.90
1	A	578	ASP	N-CA-C	-6.05	94.66	111.00
1	A	580	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	731	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	B	617	PHE	CB-CG-CD1	5.61	124.72	120.80
1	A	579	PRO	C-N-CA	5.47	135.38	121.70
1	A	578	ASP	CA-CB-CG	5.46	125.41	113.40
1	A	695	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	A	824	ASN	CA-C-O	5.27	131.17	120.10
1	B	765	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	A	605	MET	CA-CB-CG	-5.24	104.40	113.30
1	B	607	ASP	C-N-CA	5.09	134.42	121.70
1	B	787	THR	CA-CB-CG2	5.09	119.52	112.40
1	B	588	GLY	C-N-CA	5.07	134.38	121.70
1	A	622	ALA	N-CA-CB	-5.07	103.00	110.10

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

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Mol	Chain	Res	Type	Group
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 (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	2275	0	2151	176	1
1	B	2262	0	2140	115	2
2	A	35	0	0	21	0
2	B	53	0	0	14	0
All	All	4625	0	4291	275	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 31.

All (275) 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:681:GLY:HA2	2:A:59:HOH:O	1.35	1.22
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:608:ASN:HB3	1:B:612:THR:O	1.62	0.99
1:A:685:THR:HG22	2:A:53:HOH:O	1.65	0.97
1:A:605:MET:HE3	1:A:607:ASP:OD1	1.65	0.96
1:B:614:ASP:OD2	2:B:33:HOH:O	1.82	0.96
1:B:587:GLY:O	1:B:588:GLY:C	2.05	0.94
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:685:THR:C	1:A:712:ASP:O	2.06	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:HZ1	1.88	0.86
1:A:789:PRO:CB	1:A:843:LYS:NZ	2.39	0.86
1:A:605:MET:CE	1:A:607:ASP:OD1	2.24	0.85
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: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: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:B:587:GLY:C	1:B:588:GLY:O	2.21	0.78
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:B:722:PRO:HB2	2:B:86:HOH:O	1.85	0.75
1:A:789:PRO:HB3	1:A:843:LYS:HZ1	1.50	0.75
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:605:MET:HE2	1:A:607:ASP:OD2	1.89	0.73
1:A:685:THR:O	1:A:712:ASP:HA	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:566:CYS:SG	1:A:621:GLU:CD	2.70	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:HB2	1:A:843:LYS:NZ	2.09	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:B:606:VAL:CG1	1:B:614:ASP:HB2	2.28	0.64
1:A:782:PHE:HB3	1:A:856:ALA:HB3	1.80	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:B:836:VAL:O	1:B:837:LEU:HD13	1.99	0.63
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:722:PRO:C	2:B:86:HOH:O	2.38	0.61
1:B:630:THR:HB	1:B:634:ASP:N	2.10	0.61
1:B:582:VAL:CG1	2:B:17:HOH:O	2.47	0.61
1:A:845:PRO:HA	2:A:88:HOH:O	2.00	0.61
1:A:605:MET:HE2	1:A:607:ASP:CG	2.21	0.61
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:655:TYR:HA	1:A:739:LYS:HB3	1.82	0.60
1:A:629:LEU:O	1:A:636:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:685:THR:O	1:A:712:ASP:C	2.41	0.58
1:B:565:GLU:OE2	1:B:734:ARG:NH2	2.35	0.58
1:A:650:SER:HG	1:A:679:THR:HA	1.69	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:789:PRO:CG	1:A:843:LYS:NZ	2.67	0.57
1:A:677:VAL:HG13	1:A:682:VAL:O	2.05	0.57
1:A:598:PRO:HG2	1:A:622:ALA:CB	2.22	0.57
1:A:572:PHE:CZ	1:A:615:VAL:HG11	2.41	0.56
1:A:757:SER:C	1:B:765:VAL:HG12	2.25	0.56
1:B:608:ASN:ND2	1:B:610:ASP:O	2.22	0.56
1:A:661:LEU:HD13	1:A:741:MET:CE	2.35	0.56
1:A:564:GLY:HA3	1:A:645:VAL:HG22	1.87	0.56
1:A:757:SER:O	1:B:765:VAL:HG12	2.05	0.56
1:A:788:GLY:HA3	1:A:817:PHE:CE1	2.40	0.56
1:A:758:PHE:HE1	1:B:763:PHE:CD1	2.23	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
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:B:565:GLU:O	1:B:619:PRO:HG2	2.06	0.55
1:A:753:GLY:HA2	1:B:823:LEU:HB2	1.89	0.55
1:A:790:ALA:HB3	1:A:850:PHE:CZ	2.42	0.55
1:A:794:THR:O	1:A:809:TYR:HA	2.07	0.55
1:B:608:ASN:HD22	1:B:610:ASP:C	2.08	0.55
1:A:661:LEU:HD13	1:A:741:MET:HE1	1.89	0.54
1:B:814:ASN:CB	1:B:843:LYS:HB3	2.35	0.54
1:B:549:ALA:HA	1:B:577:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:A:850:PHE:N	2.75	0.54
1:A:579:PRO:HG3	2:A:14:HOH:O	1.77	0.54
1:A:566:CYS:HG	1:A:647:PRO:HA	1.73	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: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:B:577:VAL:HG13	1:B:580:ASP:N	2.22	0.53
1:A:835:GLN:HA	1:B:834:LYS:O	2.08	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:A:789:PRO:CG	1:A:843:LYS:HZ1	2.23	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:674:ILE:HD13	1:A:674:ILE:N	2.25	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: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:577:VAL:HG12	1:A:580:ASP:CA	2.41	0.51
1:A:568:GLN:C	1:A:618:GLU:HG3	2.30	0.51
1:B:655:TYR:CD1	1:B:655:TYR:N	2.79	0.50
1:A:774:VAL:HG12	1:A:775:LYS:O	2.12	0.50
1:B:701:LEU:HD12	1:B:702:VAL:H	1.77	0.50
1:B:565:GLU:O	1:B:645:VAL:HG13	2.12	0.50
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:B:606:VAL:C	1:B:607:ASP:O	2.49	0.49
1:A:639:PHE:HB3	1:A:640:PRO:CA	2.41	0.49
1:B:762:THR:HA	1:B:807:ALA:O	2.12	0.49
1:A:709:ASP:OD1	1:A:711:ASN:CG	2.50	0.49
1:B:799:ASP:C	1:B:801:GLN:H	2.15	0.49
1:A:691:PHE:CE1	1:A:733:LEU:HD13	2.48	0.49
1:A:566:CYS:HB2	1:A:648:ALA:HB2	1.93	0.49
1:A:577:VAL:HG12	1:A:580:ASP:C	2.33	0.49
1:A:784:VAL:HG21	1:A:807:ALA:HB2	1.95	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:796:ASP:O	1:B:807:ALA:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:PRO:HG3	1:B:645:VAL:CG2	2.44	0.48
1:B:572:PHE:CE2	1:B:615:VAL:HG11	2.48	0.48
1:A:721:ALA:HB1	1:A:727:TYR:CZ	2.49	0.48
1:A:582:VAL:HG21	1:A:586:ASP:OD2	2.14	0.48
1:B:720:ASP:O	1:B:722:PRO:HD3	2.14	0.47
1:B:572:PHE:CE2	1:B:615:VAL:CG1	2.97	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: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:CD1	1:A:741:MET:CE	2.93	0.47
1:A:661:LEU:HD21	1:A:672:PHE:CD2	2.50	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:B:565:GLU:CD	1:B:568:GLN:HG3	2.35	0.47
1:B:667:ASN:OD1	1:B:750:GLY:HA3	2.15	0.47
1:B:608:ASN:CG	1:B:612:THR:O	2.54	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:661:LEU:CD1	1:A:741:MET:HE1	2.45	0.46
1:A:789:PRO:CB	1:A:843:LYS:HZ3	2.27	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:577:VAL:HG13	1:B:580:ASP:H	1.81	0.46
1:B:570:SER:O	1:B:616:GLU:HA	2.16	0.46
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:A:789:PRO:HB2	1:A:843:LYS:HZ3	1.81	0.46
1:B:739:LYS:HG2	1:B:740:ASN:ND2	2.31	0.46
1:B:582:VAL:HG21	1:B:586:ASP:OD2	2.16	0.45
1:A:828:ILE:HA	1:B:753:GLY:O	2.17	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: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:620:LYS:HB3	2:B:8:HOH:O	2.15	0.45
1:B:793:ILE:HA	1:B:810:SER:O	2.16	0.45
1:B:639:PHE:HB3	1:B:640:PRO:HA	1.97	0.45
1:A:682:VAL:HG12	1:A:683:ALA:N	2.31	0.44
1:B:639:PHE:HA	1:B:640:PRO:C	2.38	0.44
1:B:831:SER:HA	1:B:832:PRO:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:GLY:C	1:A:599:ALA:H	2.19	0.44
1:B:854:ARG:HG2	1:B:854:ARG:NH1	2.27	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:A:551:PRO:HG3	1:A:631:LEU:HD23	2.00	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:574:ILE:HD13	1:B:629:LEU:HD11	2.01	0.43
1:A:699:ASP:O	1:A:699:ASP:CG	2.57	0.43
1:A:731:VAL:CG1	1:A:738:ILE:HD11	2.49	0.43
1:A:672:PHE:CD1	1:A:672:PHE:C	2.92	0.43
1:A:790:ALA:HB3	1:A:850:PHE:HZ	1.84	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:591:PHE:CD2	1:B:613:TYR:CZ	3.07	0.42
1:A:552:GLU:O	1:A:637:ASN:HB2	2.20	0.42
1:A:831:SER:HA	1:A:832:PRO:C	2.40	0.42
1:A:605:MET:HE2	1:A:607:ASP:OD1	2.09	0.42
1:A:845:PRO:C	1:A:847:VAL:H	2.22	0.42
1:B:629:LEU:HD13	1:B:636:VAL:HB	2.02	0.42
1:A:577:VAL:HG12	1:A:580:ASP:N	2.35	0.42
1:B:722:PRO:HG2	2:B:86:HOH:O	2.20	0.42
1:A:684:ARG:O	1:A:712:ASP:O	2.38	0.42
1:A:624:ASP:CG	1:A:644:THR:HG22	2.40	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:A:789:PRO:CG	1:A:843:LYS:HZ3	2.34	0.41
1:B:800:ASN:HB2	1:B:804:THR:OG1	2.19	0.41
1:B:653:HIS:HB3	1:B:677:VAL:HG11	2.01	0.41
1:A:762:THR:HA	1:A:807:ALA:O	2.20	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:566:CYS:HB3	1:A:621:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:HG22	1:A:634:ASP:O	2.21	0.41
1:A:636:VAL:C	1:A:638:GLY:H	2.23	0.41
1:A:684:ARG:NH1	1:A:684:ARG:HB3	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:B:582:VAL:HB	1:B:586:ASP:OD2	2.21	0.41
1:A:582:VAL:HG12	1:A:611:GLY:HA3	2.02	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:710:ASN:HB2	1:B:714:THR:O	2.21	0.41
1:B:689:ASP:HA	1:B:690:PRO:HD3	1.83	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:B:572:PHE:CZ	1:B:615:VAL:HG11	2.56	0.40
1:A:555:TYR:H	1:A:555:TYR:HD1	1.66	0.40
1:B:619:PRO:HG3	1:B:645:VAL:HG21	2.04	0.40
1:B:565:GLU:C	1:B:645:VAL:HG13	2.42	0.40
1:B:715:TYR:CD1	1:B:715:TYR:N	2.90	0.40
1:A:789:PRO:HG2	1:A:843:LYS:HZ3	1.86	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 (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	304/311 (98%)	252 (83%)	35 (12%)	17 (6%)	2 6
1	B	302/311 (97%)	256 (85%)	32 (11%)	14 (5%)	3 9
All	All	606/622 (97%)	508 (84%)	67 (11%)	31 (5%)	2 8

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
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 (i)

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%)	216 (89%)	27 (11%)	8 23
1	B	241/247 (98%)	207 (86%)	34 (14%)	4 12
All	All	484/494 (98%)	423 (87%)	61 (13%)	5 17

All (61) 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	596	GLU
1	A	607	ASP
1	A	629	LEU
1	A	630	THR
1	A	631	LEU
1	A	653	HIS
1	A	674	ILE
1	A	701	LEU
1	A	702	VAL
1	A	747	CYS
1	A	757	SER
1	A	771	LYS
1	A	775	LYS
1	A	776	THR
1	A	785	SER
1	A	796	ASP
1	A	811	LEU
1	A	818	SER
1	A	837	LEU
1	A	844	ASN
1	A	850	PHE

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Mol	Chain	Res	Type
1	B	550	ASP
1	B	552	GLU
1	B	578	ASP
1	B	593	VAL
1	B	620	LYS
1	B	626	VAL
1	B	629	LEU
1	B	631	LEU
1	B	634	ASP
1	B	642	THR
1	B	643	VAL
1	B	652	GLU
1	B	663	LYS
1	B	666	ASP
1	B	704	ASP
1	B	706	LYS
1	B	743	ILE
1	B	748	ILE
1	B	765	VAL
1	B	771	LYS
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	842	LYS
1	B	843	LYS
1	B	847	VAL
1	B	848	LYS
1	B	849	SER
1	B	853	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	827	HIS
1	B	575	HIS
1	B	653	HIS
1	B	740	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 carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.