



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:40 am GMT

PDB ID : 1ND7
Title : Conformational Flexibility Underlies Ubiquitin Ligation Mediated by the WWP1 HECT domain E3 Ligase
Authors : Verdecia, M.A.; Joaziero, C.A.P.; Wells, N.J.; Ferrer, J.-L.; Bowman, M.E.; Hunter, T.; Noel, J.P.
Deposited on : 2002-12-08
Resolution : 2.10 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
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

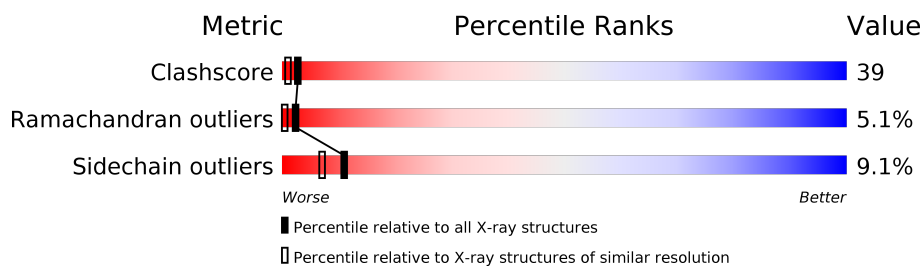
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	 55% 34% 7% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3118 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 WW domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			3118	2018	520	559	21			

There are 2 discrepancies between the modelled and reference sequences:

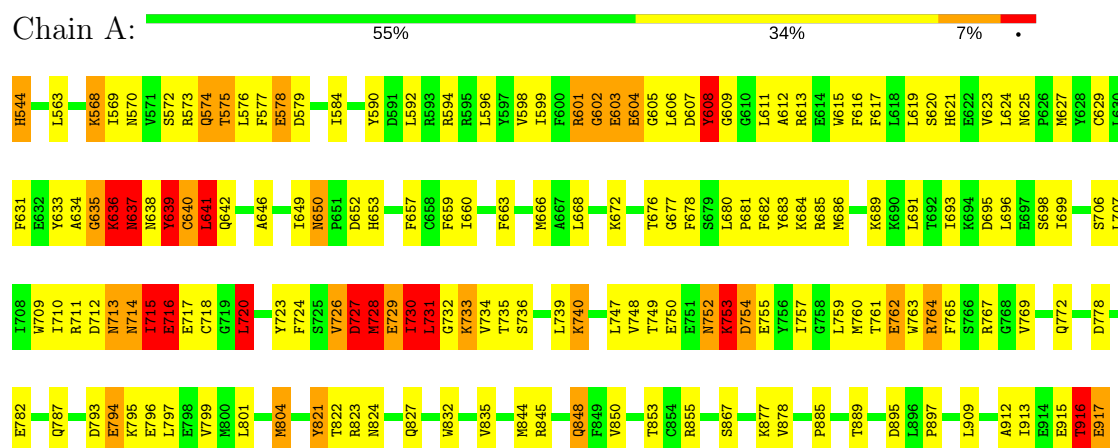
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	HIS	-	EXPRESSION TAG	UNP Q9H0M0
A	545	MET	-	initiator Methionine	UNP Q9H0M0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: WW domain-containing protein 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.20Å 50.85Å 58.43Å 113.47° 99.21° 102.26°	Depositor
Resolution (Å)	32.08 – 2.10	Depositor
% Data completeness (in resolution range)	94.2 (32.08-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3118	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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	0.75	9/3201 (0.3%)	1.06	37/4320 (0.9%)

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	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	916	THR	CA-C	9.73	1.78	1.52
1	A	916	THR	CA-CB	7.65	1.73	1.53
1	A	729	GLU	N-CA	7.40	1.61	1.46
1	A	728	MET	N-CA	6.99	1.60	1.46
1	A	637	ASN	N-CA	-6.51	1.33	1.46
1	A	734	VAL	CA-CB	6.15	1.67	1.54
1	A	916	THR	N-CA	6.14	1.58	1.46
1	A	917	GLU	CA-C	5.45	1.67	1.52
1	A	730	ILE	N-CA	5.24	1.56	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	GLY	O-C-N	14.17	145.38	122.70
1	A	727	ASP	CB-CA-C	11.99	134.38	110.40
1	A	917	GLU	N-CA-CB	11.72	131.70	110.60
1	A	716	GLU	O-C-N	11.51	141.12	122.70
1	A	636	LYS	O-C-N	11.18	140.59	122.70
1	A	717	GLU	CB-CA-C	10.31	131.03	110.40
1	A	602	GLY	CA-C-N	-9.38	96.56	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	LYS	CA-C-N	-8.85	97.73	117.20
1	A	716	GLU	CA-C-N	-8.55	98.39	117.20
1	A	639	TYR	N-CA-C	8.51	133.98	111.00
1	A	727	ASP	C-N-CA	8.07	141.87	121.70
1	A	727	ASP	O-C-N	7.76	135.11	122.70
1	A	601	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	A	916	THR	N-CA-C	7.59	131.51	111.00
1	A	726	VAL	O-C-N	7.31	134.39	122.70
1	A	727	ASP	N-CA-CB	-7.09	97.84	110.60
1	A	636	LYS	CB-CA-C	-6.59	97.22	110.40
1	A	613	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	A	916	THR	CA-C-O	-6.53	106.39	120.10
1	A	916	THR	CA-C-N	-6.08	103.83	117.20
1	A	639	TYR	C-N-CA	-6.07	106.53	121.70
1	A	728	MET	CG-SD-CE	6.04	109.87	100.20
1	A	640	CYS	C-N-CA	-6.04	106.60	121.70
1	A	608	TYR	N-CA-C	5.76	126.56	111.00
1	A	720	LEU	CB-CA-C	-5.76	99.26	110.20
1	A	715	ILE	N-CA-C	5.59	126.10	111.00
1	A	635	GLY	O-C-N	5.53	131.54	122.70
1	A	602	GLY	N-CA-C	-5.50	99.34	113.10
1	A	917	GLU	N-CA-C	-5.42	96.36	111.00
1	A	726	VAL	CA-C-N	-5.39	105.33	117.20
1	A	716	GLU	C-N-CA	5.35	135.08	121.70
1	A	727	ASP	CA-C-N	-5.34	105.45	117.20
1	A	728	MET	N-CA-C	5.30	125.31	111.00
1	A	601	ARG	CB-CA-C	5.24	120.87	110.40
1	A	716	GLU	N-CA-C	5.16	124.94	111.00
1	A	602	GLY	C-N-CA	5.08	134.40	121.70
1	A	641	LEU	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	THR	Mainchain,Peptide

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	3118	0	3046	240	0
All	All	3118	0	3046	240	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 39.

All (240) 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:728:MET:CE	1:A:735:THR:HG23	1.24	1.57
1:A:916:THR:CA	1:A:916:THR:C	1.78	1.51
1:A:728:MET:CE	1:A:735:THR:CG2	1.85	1.50
1:A:570:ASN:OD1	1:A:601:ARG:HD3	1.28	1.33
1:A:640:CYS:HB3	1:A:677:GLY:O	1.28	1.32
1:A:636:LYS:HG2	1:A:637:ASN:OD1	1.21	1.31
1:A:570:ASN:HB3	1:A:601:ARG:NE	1.45	1.30
1:A:728:MET:HE1	1:A:735:THR:CG2	1.50	1.30
1:A:728:MET:HE3	1:A:735:THR:CG2	1.52	1.28
1:A:570:ASN:CB	1:A:601:ARG:HE	1.52	1.22
1:A:749:THR:OG1	1:A:752:ASN:ND2	1.78	1.15
1:A:728:MET:HE3	1:A:735:THR:HG21	1.32	1.11
1:A:636:LYS:O	1:A:638:ASN:N	1.87	1.08
1:A:752:ASN:H	1:A:752:ASN:ND2	1.36	1.06
1:A:822:THR:HG22	1:A:824:ASN:H	1.19	1.05
1:A:601:ARG:C	1:A:603:GLU:H	1.42	1.05
1:A:640:CYS:SG	1:A:855:ARG:NH1	2.31	1.03
1:A:601:ARG:HB2	1:A:601:ARG:HH11	1.23	1.03
1:A:636:LYS:CG	1:A:637:ASN:OD1	2.08	1.01
1:A:570:ASN:OD1	1:A:601:ARG:CD	2.11	0.99
1:A:752:ASN:HD22	1:A:752:ASN:N	1.55	0.99
1:A:601:ARG:NH1	1:A:601:ARG:HB2	1.81	0.96
1:A:570:ASN:CG	1:A:601:ARG:HD3	1.84	0.96
1:A:749:THR:N	1:A:752:ASN:OD1	1.97	0.96
1:A:795:LYS:NZ	1:A:916:THR:HG21	1.79	0.96
1:A:684:LYS:HG3	1:A:794:GLU:HG2	1.47	0.94
1:A:728:MET:HE1	1:A:735:THR:HG22	1.44	0.94
1:A:568:LYS:H	1:A:568:LYS:HE2	1.33	0.94
1:A:601:ARG:C	1:A:603:GLU:N	2.23	0.91
1:A:795:LYS:NZ	1:A:916:THR:CG2	2.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:MET:HE1	1:A:735:THR:HG23	1.03	0.89
1:A:795:LYS:HZ2	1:A:916:THR:CG2	1.85	0.89
1:A:572:SER:HB2	1:A:575:THR:HG22	1.53	0.89
1:A:726:VAL:C	1:A:727:ASP:OD2	2.13	0.87
1:A:636:LYS:C	1:A:638:ASN:H	1.77	0.87
1:A:624:LEU:HD21	1:A:676:THR:HA	1.55	0.87
1:A:602:GLY:O	1:A:604:GLU:HG3	1.74	0.86
1:A:640:CYS:CB	1:A:677:GLY:O	2.21	0.86
1:A:696:LEU:HD11	1:A:761:THR:HG22	1.55	0.85
1:A:601:ARG:CB	1:A:601:ARG:HH11	1.90	0.84
1:A:729:GLU:HG2	1:A:730:ILE:H	1.43	0.84
1:A:616:PHE:O	1:A:620:SER:HB2	1.79	0.83
1:A:636:LYS:C	1:A:638:ASN:N	2.27	0.80
1:A:640:CYS:HB3	1:A:677:GLY:C	2.03	0.79
1:A:752:ASN:HD22	1:A:752:ASN:H	0.81	0.79
1:A:727:ASP:N	1:A:727:ASP:OD2	2.16	0.78
1:A:728:MET:SD	1:A:735:THR:HG23	2.24	0.78
1:A:750:GLU:HA	1:A:753:LYS:NZ	1.99	0.78
1:A:684:LYS:CG	1:A:794:GLU:HG2	2.14	0.78
1:A:570:ASN:HD21	1:A:599:ILE:HD11	1.49	0.76
1:A:607:ASP:OD1	1:A:608:TYR:N	2.18	0.76
1:A:728:MET:CE	1:A:735:THR:HG22	2.06	0.76
1:A:570:ASN:HB3	1:A:601:ARG:HE	0.65	0.74
1:A:715:ILE:HG22	1:A:715:ILE:O	1.87	0.73
1:A:715:ILE:O	1:A:715:ILE:CG2	2.37	0.73
1:A:568:LYS:H	1:A:568:LYS:CE	2.03	0.72
1:A:757:ILE:O	1:A:761:THR:HG23	1.89	0.72
1:A:821:TYR:HE2	1:A:827:GLN:HG3	1.56	0.70
1:A:795:LYS:HZ1	1:A:916:THR:HG21	1.53	0.70
1:A:916:THR:CA	1:A:917:GLU:N	2.53	0.70
1:A:639:TYR:HD2	1:A:639:TYR:O	1.73	0.70
1:A:649:ILE:HG13	1:A:650:ASN:H	1.58	0.69
1:A:709:TRP:O	1:A:713:ASN:HB3	1.93	0.69
1:A:750:GLU:HA	1:A:753:LYS:HZ3	1.57	0.69
1:A:804:MET:HG3	1:A:844:MET:SD	2.32	0.69
1:A:752:ASN:O	1:A:754:ASP:N	2.27	0.68
1:A:752:ASN:N	1:A:752:ASN:ND2	2.17	0.68
1:A:821:TYR:CE2	1:A:827:GLN:HG3	2.29	0.68
1:A:749:THR:CB	1:A:752:ASN:HD21	2.07	0.67
1:A:750:GLU:HA	1:A:753:LYS:CE	2.24	0.67
1:A:592:LEU:HD23	1:A:666:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:TYR:CD2	1:A:639:TYR:O	2.48	0.66
1:A:731:LEU:HD12	1:A:733:LYS:HD2	1.77	0.66
1:A:726:VAL:CA	1:A:727:ASP:OD2	2.43	0.66
1:A:912:ALA:O	1:A:916:THR:HB	1.95	0.65
1:A:728:MET:HE3	1:A:735:THR:HG23	1.24	0.65
1:A:764:ARG:O	1:A:764:ARG:HD3	1.97	0.65
1:A:575:THR:HG23	1:A:579:ASP:OD1	1.98	0.64
1:A:916:THR:O	1:A:916:THR:CA	2.43	0.64
1:A:636:LYS:HG2	1:A:637:ASN:CG	2.14	0.64
1:A:649:ILE:HG13	1:A:650:ASN:N	2.12	0.64
1:A:731:LEU:HB3	1:A:733:LYS:HE3	1.79	0.64
1:A:916:THR:HA	1:A:916:THR:C	2.06	0.64
1:A:715:ILE:O	1:A:716:GLU:CG	2.46	0.63
1:A:749:THR:H	1:A:752:ASN:CG	1.97	0.63
1:A:764:ARG:NH1	1:A:767:ARG:HH12	1.96	0.63
1:A:635:GLY:O	1:A:636:LYS:HB2	1.98	0.63
1:A:572:SER:HB2	1:A:575:THR:CG2	2.27	0.62
1:A:570:ASN:CB	1:A:601:ARG:NE	2.28	0.62
1:A:578:GLU:CD	1:A:578:GLU:H	2.03	0.62
1:A:698:SER:C	1:A:699:ILE:HD12	2.20	0.61
1:A:714:ASN:HD22	1:A:715:ILE:N	1.97	0.61
1:A:731:LEU:HB3	1:A:733:LYS:CD	2.30	0.61
1:A:731:LEU:HB3	1:A:733:LYS:HD2	1.81	0.61
1:A:795:LYS:HZ2	1:A:916:THR:HG21	1.55	0.61
1:A:570:ASN:ND2	1:A:599:ILE:HD11	2.14	0.61
1:A:885:PRO:HG2	1:A:912:ALA:CB	2.31	0.61
1:A:544:HIS:HB3	1:A:845:ARG:CD	2.31	0.60
1:A:607:ASP:OD1	1:A:608:TYR:HA	2.01	0.60
1:A:795:LYS:HZ1	1:A:916:THR:CG2	2.10	0.60
1:A:832:TRP:O	1:A:835:VAL:HG22	2.02	0.60
1:A:730:ILE:O	1:A:731:LEU:HB2	2.01	0.59
1:A:778:ASP:O	1:A:782:GLU:HG3	2.02	0.59
1:A:682:PHE:CE1	1:A:686:MET:HE2	2.37	0.59
1:A:733:LYS:N	1:A:733:LYS:HD3	2.18	0.59
1:A:619:LEU:HD23	1:A:663:PHE:CE2	2.37	0.59
1:A:584:ILE:HD12	1:A:659:PHE:HE1	1.67	0.59
1:A:570:ASN:CG	1:A:601:ARG:CD	2.65	0.58
1:A:570:ASN:OD1	1:A:599:ILE:HG13	2.02	0.58
1:A:747:LEU:HD13	1:A:748:VAL:N	2.18	0.58
1:A:750:GLU:HA	1:A:753:LYS:HE2	1.84	0.58
1:A:572:SER:CB	1:A:575:THR:HG22	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:CYS:O	1:A:718:CYS:SG	2.60	0.58
1:A:715:ILE:O	1:A:716:GLU:HG3	2.04	0.58
1:A:767:ARG:HG2	1:A:767:ARG:HH11	1.70	0.57
1:A:682:PHE:HE1	1:A:686:MET:HE2	1.69	0.57
1:A:696:LEU:CD1	1:A:761:THR:HG22	2.29	0.57
1:A:731:LEU:HB3	1:A:733:LYS:CE	2.35	0.57
1:A:620:SER:O	1:A:624:LEU:HB2	2.05	0.57
1:A:623:VAL:HG23	1:A:624:LEU:HD13	1.86	0.56
1:A:715:ILE:O	1:A:716:GLU:OE2	2.23	0.56
1:A:623:VAL:HG23	1:A:624:LEU:CD1	2.36	0.56
1:A:822:THR:HG22	1:A:824:ASN:N	2.04	0.55
1:A:569:ILE:HD12	1:A:596:LEU:HD11	1.89	0.55
1:A:570:ASN:HB3	1:A:601:ARG:CD	2.32	0.55
1:A:764:ARG:CZ	1:A:767:ARG:HH12	2.20	0.55
1:A:621:HIS:O	1:A:625:ASN:HB2	2.08	0.54
1:A:714:ASN:HD21	1:A:750:GLU:CD	2.11	0.54
1:A:616:PHE:CE1	1:A:672:LYS:HG3	2.42	0.53
1:A:619:LEU:O	1:A:623:VAL:HG22	2.08	0.53
1:A:832:TRP:HE3	1:A:835:VAL:HG21	1.74	0.53
1:A:598:VAL:HG13	1:A:611:LEU:HB3	1.89	0.53
1:A:631:PHE:HE1	1:A:660:ILE:HD13	1.74	0.53
1:A:568:LYS:N	1:A:568:LYS:HE2	2.14	0.53
1:A:726:VAL:N	1:A:727:ASP:OD2	2.41	0.53
1:A:577:PHE:CE1	1:A:623:VAL:HG12	2.43	0.53
1:A:624:LEU:HG	1:A:641:LEU:HD21	1.91	0.52
1:A:680:LEU:N	1:A:681:PRO:HD2	2.24	0.52
1:A:885:PRO:HG2	1:A:912:ALA:HB2	1.90	0.52
1:A:712:ASP:O	1:A:713:ASN:HB2	2.08	0.52
1:A:624:LEU:CD2	1:A:676:THR:HA	2.34	0.52
1:A:850:VAL:O	1:A:889:THR:HA	2.10	0.52
1:A:794:GLU:H	1:A:794:GLU:CD	2.13	0.51
1:A:570:ASN:CB	1:A:601:ARG:CD	2.87	0.51
1:A:577:PHE:HE1	1:A:623:VAL:HG12	1.75	0.51
1:A:696:LEU:CD1	1:A:707:LEU:HD12	2.41	0.51
1:A:750:GLU:CB	1:A:753:LYS:HZ1	2.23	0.51
1:A:563:LEU:HD12	1:A:590:TYR:O	2.11	0.51
1:A:750:GLU:CA	1:A:753:LYS:NZ	2.72	0.51
1:A:598:VAL:HG13	1:A:598:VAL:O	2.10	0.51
1:A:668:LEU:HG	1:A:801:LEU:HD21	1.92	0.51
1:A:570:ASN:O	1:A:601:ARG:NH2	2.40	0.50
1:A:832:TRP:CE3	1:A:835:VAL:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:CYS:HB3	1:A:677:GLY:CA	2.41	0.50
1:A:787:GLN:NE2	1:A:787:GLN:HA	2.27	0.50
1:A:570:ASN:OD1	1:A:601:ARG:CG	2.59	0.50
1:A:763:TRP:O	1:A:767:ARG:HB3	2.12	0.50
1:A:598:VAL:HG11	1:A:611:LEU:O	2.12	0.49
1:A:750:GLU:HB3	1:A:753:LYS:HZ1	1.76	0.49
1:A:769:VAL:HA	1:A:772:GLN:OE1	2.13	0.49
1:A:909:LEU:O	1:A:913:ILE:HG13	2.12	0.49
1:A:729:GLU:HG2	1:A:730:ILE:N	2.21	0.49
1:A:607:ASP:O	1:A:608:TYR:HB3	2.13	0.49
1:A:695:ASP:O	1:A:699:ILE:HD13	2.13	0.49
1:A:574:GLN:OE1	1:A:574:GLN:HA	2.13	0.49
1:A:749:THR:CA	1:A:752:ASN:HD21	2.25	0.49
1:A:650:ASN:ND2	1:A:652:ASP:H	2.11	0.49
1:A:733:LYS:H	1:A:733:LYS:HD3	1.78	0.49
1:A:544:HIS:HB3	1:A:845:ARG:HD2	1.93	0.48
1:A:646:ALA:O	1:A:649:ILE:HG12	2.13	0.48
1:A:650:ASN:HD22	1:A:650:ASN:C	2.16	0.48
1:A:844:MET:O	1:A:848:GLN:HG2	2.13	0.48
1:A:623:VAL:HG23	1:A:624:LEU:N	2.29	0.48
1:A:735:THR:OG1	1:A:736:SER:N	2.47	0.48
1:A:641:LEU:H	1:A:641:LEU:HD12	1.79	0.47
1:A:544:HIS:HB3	1:A:845:ARG:NE	2.29	0.47
1:A:714:ASN:ND2	1:A:750:GLU:HG2	2.30	0.47
1:A:544:HIS:N	1:A:544:HIS:CD2	2.83	0.47
1:A:767:ARG:HG3	1:A:767:ARG:O	2.15	0.47
1:A:599:ILE:O	1:A:599:ILE:HG13	2.15	0.47
1:A:640:CYS:SG	1:A:855:ARG:CZ	3.03	0.46
1:A:750:GLU:CB	1:A:753:LYS:NZ	2.78	0.46
1:A:584:ILE:HD11	1:A:615:TRP:HH2	1.79	0.46
1:A:740:LYS:HB2	1:A:740:LYS:NZ	2.30	0.46
1:A:625:ASN:OD1	1:A:627:MET:HG2	2.14	0.46
1:A:730:ILE:O	1:A:730:ILE:HG23	2.15	0.46
1:A:749:THR:C	1:A:752:ASN:HD21	2.18	0.46
1:A:731:LEU:HD13	1:A:732:GLY:N	2.31	0.46
1:A:878:VAL:HG21	1:A:895:ASP:HB3	1.98	0.46
1:A:636:LYS:HZ1	1:A:867:SER:C	2.20	0.45
1:A:568:LYS:H	1:A:568:LYS:CD	2.29	0.45
1:A:715:ILE:O	1:A:716:GLU:CD	2.54	0.45
1:A:764:ARG:CZ	1:A:767:ARG:NH1	2.79	0.45
1:A:570:ASN:CA	1:A:601:ARG:HE	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LEU:HD12	1:A:592:LEU:N	2.32	0.45
1:A:748:VAL:HA	1:A:752:ASN:OD1	2.17	0.45
1:A:683:TYR:CE2	1:A:686:MET:HE1	2.52	0.45
1:A:691:LEU:HD13	1:A:765:PHE:CD1	2.52	0.45
1:A:689:LYS:HE3	1:A:793:ASP:HA	1.98	0.44
1:A:822:THR:CG2	1:A:823:ARG:N	2.80	0.44
1:A:693:ILE:O	1:A:696:LEU:HB2	2.17	0.44
1:A:636:LYS:HB3	1:A:637:ASN:CB	2.46	0.44
1:A:759:LEU:O	1:A:762:GLU:HG3	2.17	0.44
1:A:666:MET:HB2	1:A:666:MET:HE2	1.80	0.43
1:A:570:ASN:CB	1:A:601:ARG:HD3	2.49	0.43
1:A:601:ARG:HA	1:A:603:GLU:HG3	2.00	0.43
1:A:636:LYS:CB	1:A:637:ASN:OD1	2.64	0.43
1:A:678:PHE:HB2	1:A:683:TYR:CZ	2.54	0.43
1:A:853:THR:OG1	1:A:855:ARG:HG2	2.17	0.43
1:A:832:TRP:HA	1:A:835:VAL:HG22	2.00	0.43
1:A:739:LEU:HD11	1:A:760:MET:SD	2.59	0.43
1:A:691:LEU:HD13	1:A:765:PHE:CG	2.54	0.43
1:A:795:LYS:NZ	1:A:916:THR:HG23	2.29	0.43
1:A:636:LYS:CG	1:A:637:ASN:CG	2.82	0.42
1:A:629:CYS:CB	1:A:649:ILE:HD11	2.49	0.42
1:A:752:ASN:O	1:A:755:GLU:N	2.49	0.42
1:A:573:ARG:HD2	1:A:604:GLU:OE2	2.18	0.42
1:A:723:TYR:CZ	1:A:747:LEU:HD23	2.54	0.42
1:A:575:THR:O	1:A:578:GLU:HG2	2.20	0.42
1:A:821:TYR:CE1	1:A:877:LYS:HB2	2.54	0.42
1:A:612:ALA:O	1:A:616:PHE:HD1	2.03	0.42
1:A:617:PHE:O	1:A:620:SER:HB3	2.19	0.42
1:A:706:SER:O	1:A:710:ILE:HG13	2.19	0.42
1:A:767:ARG:HG2	1:A:767:ARG:NH1	2.33	0.42
1:A:633:TYR:OH	1:A:639:TYR:CZ	2.73	0.41
1:A:594:ARG:HG2	1:A:594:ARG:HH11	1.84	0.41
1:A:878:VAL:O	1:A:897:PRO:HA	2.20	0.41
1:A:584:ILE:HD11	1:A:615:TRP:CH2	2.56	0.41
1:A:606:LEU:N	1:A:606:LEU:HD12	2.36	0.41
1:A:598:VAL:CG1	1:A:611:LEU:HB3	2.51	0.41
1:A:699:ILE:N	1:A:699:ILE:HD12	2.36	0.41
1:A:799:VAL:HG11	1:A:804:MET:CE	2.51	0.41
1:A:607:ASP:C	1:A:608:TYR:HD2	2.24	0.41
1:A:684:LYS:HD3	1:A:691:LEU:HD23	2.04	0.40
1:A:698:SER:HB3	1:A:889:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:PHE:CD2	1:A:740:LYS:HD3	2.56	0.40
1:A:793:ASP:OD1	1:A:796:GLU:HG3	2.20	0.40
1:A:576:LEU:O	1:A:579:ASP:OD2	2.39	0.40
1:A:657:PHE:CE1	1:A:772:GLN:HG2	2.55	0.40
1:A:716:GLU:C	1:A:718:CYS:H	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	372/374 (100%)	328 (88%)	25 (7%)	19 (5%)	2 0

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	603	GLU
1	A	608	TYR
1	A	609	GLY
1	A	634	ALA
1	A	637	ASN
1	A	711	ARG
1	A	715	ILE
1	A	728	MET
1	A	730	ILE
1	A	753	LYS
1	A	605	GLY
1	A	716	GLU
1	A	731	LEU
1	A	575	THR
1	A	604	GLU
1	A	713	ASN

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Mol	Chain	Res	Type
1	A	915	GLU
1	A	636	LYS
1	A	720	LEU

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	339/339 (100%)	308 (91%)	31 (9%)	11 7

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	HIS
1	A	568	LYS
1	A	574	GLN
1	A	578	GLU
1	A	608	TYR
1	A	636	LYS
1	A	637	ASN
1	A	639	TYR
1	A	641	LEU
1	A	642	GLN
1	A	650	ASN
1	A	653	HIS
1	A	685	ARG
1	A	714	ASN
1	A	715	ILE
1	A	720	LEU
1	A	727	ASP
1	A	728	MET
1	A	731	LEU
1	A	733	LYS
1	A	740	LYS
1	A	752	ASN
1	A	753	LYS

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Mol	Chain	Res	Type
1	A	754	ASP
1	A	762	GLU
1	A	764	ARG
1	A	794	GLU
1	A	797	LEU
1	A	804	MET
1	A	821	TYR
1	A	848	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	ASN
1	A	714	ASN
1	A	745	ASN
1	A	752	ASN
1	A	787	GLN
1	A	813	GLN
1	A	888	HIS
1	A	892	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 [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

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.