



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:31 PM GMT

PDB ID : 1KO6
Title : Crystal Structure of C-terminal Autoproteolytic Domain of Nucleoporin Nup98
Authors : Hodel, A.E.; Hodel, M.R.; Griffis, E.R.; Hennig, K.A.; Ratner, G.A.; Songli, X.; Powers, M.A.
Deposited on : 2001-12-20
Resolution : 3.00 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

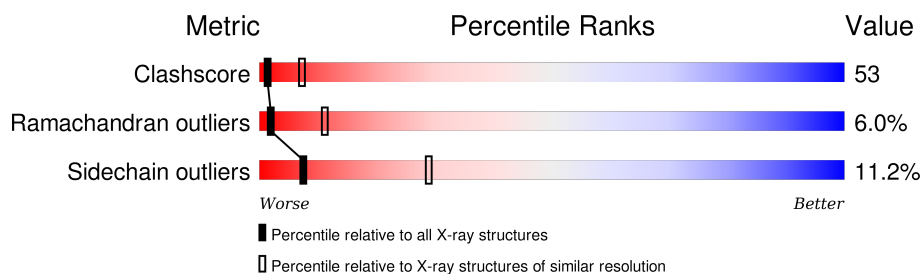
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

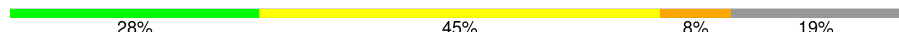



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	187	 <div>28% 45% 8% 19%</div>
1	C	187	 <div>20% 48% 10% • 21%</div>
2	B	64	 <div>9% 91%</div>
2	D	64	 <div>5% • • 91%</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2480 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 Nuclear Pore Complex Protein Nup98.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1204	762	208	231	3			
1	C	148	Total	C	N	O	S	0	0	0
			1179	748	204	224	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	MET	-	INITIATING MET	UNP P52948
C	677	MET	-	INITIATING MET	UNP P52948

- Molecule 2 is a protein called Nuclear Pore Complex Protein Nup98.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			50	32	8	10			
2	D	6	Total	C	N	O	0	0	0
			47	31	8	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	921	LEU	-	EXPRESSION TAG	UNP P52948
B	922	GLU	-	EXPRESSION TAG	UNP P52948
B	923	HIS	-	EXPRESSION TAG	UNP P52948
B	924	HIS	-	EXPRESSION TAG	UNP P52948
B	925	HIS	-	EXPRESSION TAG	UNP P52948
B	926	HIS	-	EXPRESSION TAG	UNP P52948
B	927	HIS	-	EXPRESSION TAG	UNP P52948
D	921	LEU	-	EXPRESSION TAG	UNP P52948
D	922	GLU	-	EXPRESSION TAG	UNP P52948
D	923	HIS	-	EXPRESSION TAG	UNP P52948

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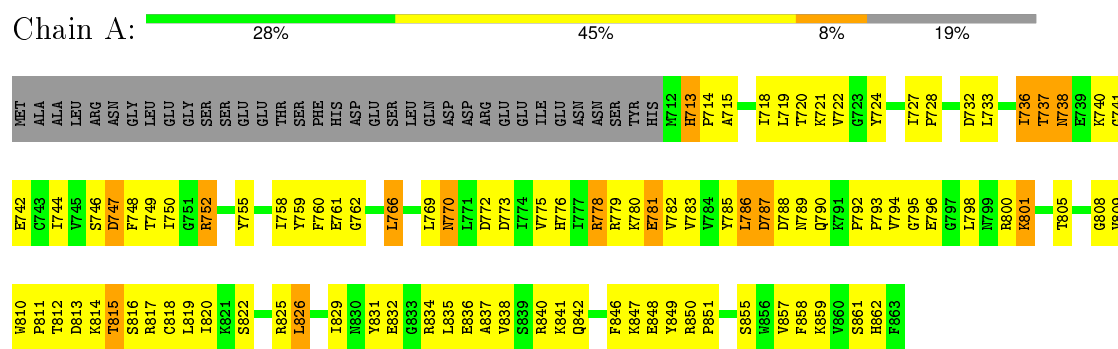
Chain	Residue	Modelled	Actual	Comment	Reference
D	924	HIS	-	EXPRESSION TAG	UNP P52948
D	925	HIS	-	EXPRESSION TAG	UNP P52948
D	926	HIS	-	EXPRESSION TAG	UNP P52948
D	927	HIS	-	EXPRESSION TAG	UNP P52948

3 Residue-property plots

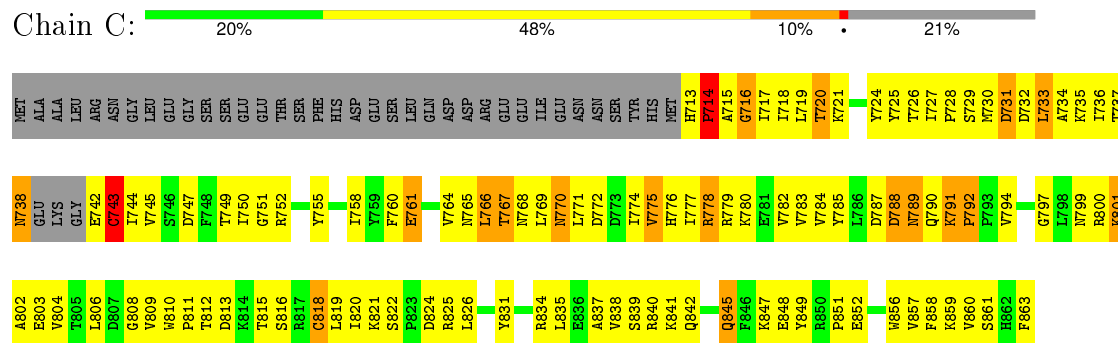
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

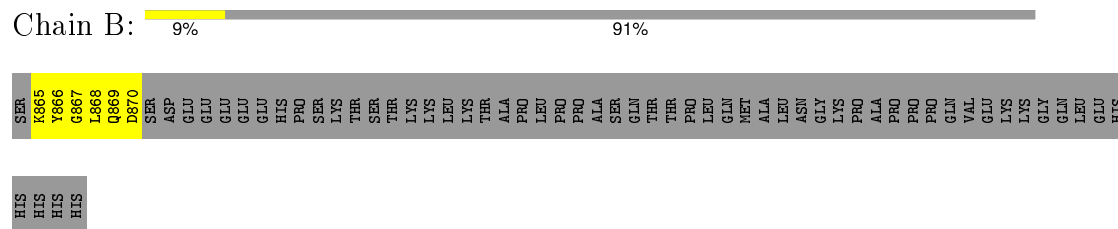
• Molecule 1: Nuclear Pore Complex Protein Nup98



• Molecule 1: Nuclear Pore Complex Protein Nup98

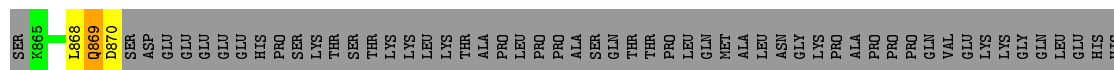


• Molecule 2: Nuclear Pore Complex Protein Nup98



• Molecule 2: Nuclear Pore Complex Protein Nup98

Chain D: 5% . . 91%

HIS
HIS
HIS

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.90Å 89.90Å 203.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2480	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	0.48	0/1229	0.69	0/1663
1	C	0.55	1/1203 (0.1%)	0.73	1/1626 (0.1%)
2	B	0.69	0/50	0.64	0/65
2	D	0.79	0/47	0.61	0/61
All	All	0.53	1/2529 (0.0%)	0.71	1/3415 (0.0%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	761	GLU	C-N	-7.30	1.20	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	761	GLU	O-C-N	-6.95	111.39	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	761	GLU	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	1204	0	1185	109	7
1	C	1179	0	1164	156	7
2	B	50	0	47	11	0
2	D	47	0	45	1	0
All	All	2480	0	2441	263	7

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 53.

All (263) 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)
2:B:870:ASP:OD2	1:C:845:GLN:NE2	1.61	1.34
1:A:847:LYS:HE3	1:A:859:LYS:HE2	1.29	1.07
1:A:812:THR:HG22	1:A:819:LEU:HD23	1.35	1.04
1:C:816:SER:OG	1:C:818:CYS:HB2	1.59	1.01
1:C:717:ILE:HD11	1:C:766:LEU:HB3	1.42	0.99
1:C:752:ARG:HD2	1:C:755:TYR:CD2	2.05	0.92
1:A:780:LYS:HG2	1:A:809:VAL:HG22	1.54	0.90
1:A:738:ASN:ND2	1:A:740:LYS:H	1.73	0.86
1:A:822:SER:HB3	1:A:825:ARG:HB2	1.57	0.86
1:A:805:THR:HG23	1:A:857:VAL:HG12	1.58	0.85
2:B:869:GLN:HG3	2:B:869:GLN:O	1.75	0.85
1:C:713:HIS:ND1	1:C:714:PRO:HD2	1.91	0.84
1:A:770:ASN:HD21	1:A:772:ASP:HB2	1.44	0.83
1:A:848:GLU:HG2	1:A:857:VAL:HG22	1.61	0.82
1:A:727:ILE:HB	1:A:749:THR:HB	1.64	0.80
1:A:848:GLU:HG2	1:A:857:VAL:CG2	2.12	0.80
1:C:750:ILE:HD13	1:C:775:VAL:HG11	1.64	0.78
1:C:766:LEU:HA	1:C:769:LEU:HD12	1.64	0.77
1:C:811:PRO:HB3	1:C:831:TYR:CE1	2.19	0.77
1:C:715:ALA:CB	1:C:743:CYS:HB2	2.14	0.77
1:A:847:LYS:HE3	1:A:859:LYS:CE	2.14	0.77
1:A:815:THR:HG23	1:A:816:SER:H	1.50	0.77
1:A:780:LYS:NZ	2:B:870:ASP:OD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:LEU:HA	1:C:772:ASP:OD1	1.87	0.74
1:C:789:ASN:OD1	1:C:790:GLN:HG3	1.86	0.74
1:C:713:HIS:HE1	1:C:734:ALA:HB2	1.52	0.72
1:A:847:LYS:HB2	1:A:857:VAL:HG23	1.71	0.72
1:C:847:LYS:HB2	1:C:857:VAL:HG23	1.71	0.71
1:C:716:GLY:O	1:C:768:ASN:HA	1.91	0.71
1:A:825:ARG:O	1:A:829:ILE:HG12	1.91	0.70
1:C:818:CYS:O	1:C:819:LEU:HB2	1.92	0.70
1:A:738:ASN:HD22	1:A:738:ASN:C	1.92	0.69
1:C:715:ALA:HB1	1:C:743:CYS:HB2	1.73	0.69
1:A:724:TYR:CE2	1:A:752:ARG:HG3	2.28	0.68
1:C:733:LEU:CD2	1:C:736:ILE:HG21	2.22	0.68
1:A:770:ASN:C	1:A:770:ASN:HD22	1.97	0.68
1:A:752:ARG:NH2	1:C:848:GLU:OE1	2.26	0.68
1:C:856:TRP:NE1	1:C:858:PHE:HD2	1.92	0.68
1:A:715:ALA:HB2	1:A:737:THR:HG21	1.77	0.67
1:C:767:THR:HG22	1:C:768:ASN:N	2.09	0.67
1:C:848:GLU:HG2	1:C:857:VAL:CG2	2.26	0.65
1:C:733:LEU:HD22	1:C:736:ILE:HG21	1.77	0.65
1:C:834:ARG:O	1:C:838:VAL:HG23	1.96	0.65
1:C:787:ASP:O	1:C:789:ASN:N	2.30	0.65
1:C:835:LEU:HD23	1:C:856:TRP:HB2	1.78	0.65
1:C:728:PRO:HG2	1:C:733:LEU:HG	1.80	0.64
1:C:790:GLN:O	1:C:792:PRO:N	2.30	0.64
1:A:715:ALA:HA	1:A:741:GLY:O	1.98	0.64
1:A:793:PRO:O	1:A:796:GLU:HB2	1.97	0.64
1:A:800:ARG:O	1:A:862:HIS:HA	1.98	0.63
1:A:770:ASN:ND2	1:A:772:ASP:HB2	2.14	0.63
1:A:733:LEU:HA	1:A:736:ILE:HG23	1.81	0.63
1:C:714:PRO:HG2	1:C:734:ALA:HB1	1.81	0.63
1:A:758:ILE:HD11	1:A:782:VAL:HG21	1.80	0.62
1:C:718:ILE:HB	1:C:770:ASN:ND2	2.14	0.62
1:A:733:LEU:O	1:A:737:THR:HG23	2.00	0.61
1:A:736:ILE:HD12	1:A:736:ILE:O	2.00	0.61
2:B:869:GLN:CG	2:B:869:GLN:O	2.45	0.60
1:C:764:VAL:HG12	1:C:766:LEU:HD13	1.84	0.60
1:C:732:ASP:C	1:C:734:ALA:H	2.06	0.60
1:A:720:THR:HB	1:A:772:ASP:OD2	2.02	0.59
1:C:815:THR:HG23	1:C:816:SER:H	1.67	0.59
1:C:839:SER:HG	1:C:856:TRP:HZ2	1.51	0.59
1:A:849:TYR:O	1:A:851:PRO:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:HIS:HB2	1:A:783:VAL:HG13	1.84	0.58
1:C:847:LYS:CE	1:C:859:LYS:HE2	2.33	0.58
1:C:745:VAL:HG13	1:C:745:VAL:O	2.04	0.58
1:C:841:LYS:HG3	1:C:842:GLN:N	2.18	0.57
1:C:838:VAL:HG12	1:C:842:GLN:HE21	1.69	0.57
1:C:838:VAL:HG12	1:C:842:GLN:NE2	2.17	0.57
1:A:801:LYS:HA	1:A:861:SER:O	2.04	0.57
1:C:733:LEU:C	1:C:736:ILE:HG22	2.25	0.56
1:A:811:PRO:HD3	1:A:831:TYR:CE2	2.39	0.56
1:A:724:TYR:CD2	1:A:752:ARG:HG3	2.40	0.56
1:C:784:VAL:HG21	1:C:863:PHE:CE2	2.41	0.56
1:A:834:ARG:O	1:A:837:ALA:HB3	2.06	0.56
1:C:848:GLU:HG2	1:C:857:VAL:HG21	1.88	0.56
1:C:717:ILE:HD11	1:C:766:LEU:CB	2.27	0.55
1:A:826:LEU:HD12	1:A:831:TYR:HB2	1.88	0.55
1:C:849:TYR:O	1:C:851:PRO:HD3	2.06	0.55
1:C:780:LYS:HA	1:C:806:LEU:HD13	1.88	0.55
1:C:733:LEU:HA	1:C:736:ILE:CG2	2.37	0.55
1:C:787:ASP:C	1:C:789:ASN:H	2.09	0.55
1:C:770:ASN:H	1:C:774:ILE:HD11	1.71	0.55
1:A:796:GLU:OE2	1:A:796:GLU:HA	2.07	0.55
1:C:776:HIS:HB2	1:C:783:VAL:CG1	2.36	0.55
1:C:770:ASN:O	1:C:774:ILE:HG13	2.07	0.54
1:C:835:LEU:CD2	1:C:856:TRP:HB2	2.37	0.54
1:C:777:ILE:HG12	1:C:782:VAL:HG23	1.89	0.54
1:A:848:GLU:HG2	1:A:857:VAL:HG21	1.89	0.54
1:A:779:ARG:HG3	1:A:780:LYS:HG3	1.89	0.54
1:A:819:LEU:HG	1:C:840:ARG:CZ	2.38	0.53
1:C:715:ALA:HB2	1:C:737:THR:CB	2.38	0.53
1:A:776:HIS:HB2	1:A:783:VAL:CG1	2.38	0.53
1:C:784:VAL:HG12	1:C:785:TYR:CD1	2.43	0.53
1:C:779:ARG:HG3	1:C:780:LYS:HG2	1.90	0.53
1:C:820:ILE:HG22	1:C:826:LEU:HD22	1.90	0.53
1:A:738:ASN:ND2	1:A:738:ASN:C	2.62	0.53
1:C:860:VAL:HG21	1:C:863:PHE:CE1	2.44	0.52
1:C:732:ASP:O	1:C:734:ALA:N	2.43	0.52
1:C:770:ASN:HD21	1:C:772:ASP:HB2	1.74	0.52
1:C:804:VAL:O	1:C:857:VAL:HA	2.10	0.52
1:A:813:ASP:OD1	1:A:816:SER:N	2.43	0.51
1:C:790:GLN:O	1:C:791:LYS:C	2.47	0.51
1:C:738:ASN:HB2	1:C:742:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:ILE:HB	1:C:770:ASN:HD22	1.73	0.51
1:A:715:ALA:HB2	1:A:737:THR:CG2	2.41	0.51
1:A:793:PRO:HD2	1:A:796:GLU:HG3	1.92	0.51
1:C:733:LEU:HD23	1:C:736:ILE:HG21	1.92	0.51
1:C:760:PHE:HB3	1:C:764:VAL:HG21	1.93	0.51
1:C:752:ARG:HD2	1:C:755:TYR:CE2	2.46	0.51
1:C:758:ILE:HD11	1:C:782:VAL:HG21	1.93	0.51
1:A:749:THR:OG1	1:A:759:TYR:HD1	1.94	0.51
1:C:847:LYS:HE3	1:C:859:LYS:HE2	1.93	0.51
1:C:810:TRP:CH2	1:C:821:LYS:HE2	2.45	0.51
1:C:733:LEU:HD21	1:C:745:VAL:HG11	1.92	0.51
1:C:813:ASP:OD1	1:C:816:SER:HB3	2.11	0.51
1:A:758:ILE:HD11	1:A:782:VAL:CG2	2.40	0.51
1:C:713:HIS:CG	1:C:714:PRO:HD2	2.46	0.50
1:C:820:ILE:O	1:C:826:LEU:HD21	2.11	0.50
1:C:731:ASP:O	1:C:732:ASP:C	2.49	0.50
1:C:770:ASN:N	1:C:774:ILE:HD11	2.26	0.50
1:A:713:HIS:CD2	1:A:715:ALA:H	2.29	0.50
1:A:836:GLU:HG3	1:A:846:PHE:CB	2.41	0.50
1:A:747:ASP:OD1	1:A:761:GLU:HG2	2.11	0.50
1:C:727:ILE:HB	1:C:749:THR:HB	1.94	0.50
1:C:787:ASP:OD2	1:C:789:ASN:HB3	2.12	0.50
1:A:738:ASN:HD22	1:A:740:LYS:H	1.53	0.50
1:C:715:ALA:HB3	1:C:743:CYS:SG	2.52	0.49
1:A:826:LEU:HD12	1:A:831:TYR:CB	2.42	0.49
1:C:718:ILE:CG2	1:C:770:ASN:ND2	2.75	0.49
1:A:733:LEU:O	1:A:736:ILE:HG23	2.12	0.49
1:C:811:PRO:HD3	1:C:831:TYR:CE2	2.48	0.49
1:A:814:LYS:O	1:A:817:ARG:HG2	2.12	0.49
1:A:847:LYS:CB	1:A:857:VAL:HG23	2.41	0.49
1:A:849:TYR:CE2	1:A:851:PRO:HG3	2.48	0.49
1:C:713:HIS:CE1	1:C:734:ALA:HB2	2.42	0.49
1:C:720:THR:N	1:C:772:ASP:OD1	2.43	0.49
1:C:845:GLN:HB2	1:C:859:LYS:HB2	1.95	0.49
1:C:760:PHE:CD1	1:C:802:ALA:HB2	2.48	0.49
1:A:718:ILE:HB	1:A:770:ASN:HA	1.94	0.48
1:C:715:ALA:O	1:C:767:THR:O	2.31	0.48
1:C:784:VAL:O	1:C:785:TYR:HB2	2.13	0.48
1:A:842:GLN:NE2	2:B:867:GLY:O	2.46	0.48
1:C:728:PRO:HB2	1:C:732:ASP:HB2	1.95	0.48
1:A:801:LYS:CA	1:A:861:SER:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:LEU:HA	1:C:769:LEU:CD1	2.38	0.48
1:C:839:SER:OG	1:C:856:TRP:CZ2	2.67	0.48
1:C:744:ILE:HG12	1:C:765:ASN:HA	1.95	0.48
1:C:839:SER:OG	1:C:856:TRP:HZ2	1.96	0.48
1:C:848:GLU:HG2	1:C:857:VAL:HG22	1.96	0.48
1:A:722:VAL:HG13	1:C:852:GLU:CD	2.34	0.47
1:A:733:LEU:HA	1:A:736:ILE:CG2	2.43	0.47
1:C:717:ILE:HG22	1:C:730:MET:CE	2.45	0.47
1:A:816:SER:OG	1:A:818:CYS:HB2	2.14	0.47
1:C:787:ASP:C	1:C:789:ASN:N	2.67	0.47
1:A:776:HIS:NE2	1:A:786:LEU:HD21	2.29	0.47
1:A:752:ARG:HD2	1:A:755:TYR:CD2	2.49	0.47
1:C:731:ASP:O	1:C:734:ALA:N	2.45	0.47
1:C:782:VAL:HB	1:C:806:LEU:HD21	1.96	0.47
1:C:847:LYS:HE3	1:C:859:LYS:NZ	2.30	0.47
1:C:721:LYS:HE3	1:C:772:ASP:HA	1.96	0.47
1:C:721:LYS:CE	1:C:772:ASP:O	2.62	0.47
1:C:736:ILE:HG23	1:C:737:THR:N	2.30	0.47
1:A:738:ASN:ND2	1:A:740:LYS:N	2.54	0.47
1:C:721:LYS:HE3	1:C:772:ASP:O	2.15	0.47
1:C:826:LEU:HD12	1:C:831:TYR:CB	2.45	0.47
1:C:766:LEU:HD12	1:C:769:LEU:HD12	1.97	0.47
1:C:790:GLN:O	1:C:792:PRO:CD	2.63	0.47
1:C:837:ALA:O	1:C:840:ARG:N	2.48	0.46
1:A:842:GLN:OE1	2:B:866:TYR:HA	2.16	0.46
1:C:778:ARG:O	1:C:779:ARG:C	2.53	0.46
2:B:870:ASP:CG	1:C:845:GLN:NE2	2.57	0.46
1:A:850:ARG:HH12	1:A:857:VAL:HG11	1.80	0.46
1:A:818:CYS:O	1:A:819:LEU:HB2	2.15	0.46
1:A:733:LEU:CA	1:A:736:ILE:HG23	2.45	0.46
1:A:728:PRO:HB2	1:A:732:ASP:HB2	1.98	0.46
1:C:733:LEU:HA	1:C:736:ILE:HG22	1.97	0.46
1:A:826:LEU:HD13	1:A:829:ILE:HD11	1.98	0.46
1:A:858:PHE:CZ	2:B:866:TYR:HB3	2.50	0.46
1:A:770:ASN:C	1:A:770:ASN:ND2	2.68	0.46
1:A:813:ASP:OD1	1:A:815:THR:HG23	2.16	0.46
1:C:764:VAL:HG23	1:C:800:ARG:HH11	1.80	0.45
1:C:856:TRP:NE1	1:C:858:PHE:CD2	2.79	0.45
1:C:785:TYR:CE2	1:C:792:PRO:HD3	2.51	0.45
1:A:760:PHE:CZ	1:A:798:LEU:HG	2.52	0.45
1:C:784:VAL:HB	1:C:863:PHE:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:PHE:CE1	1:A:766:LEU:HD21	2.51	0.45
1:A:770:ASN:ND2	1:A:773:ASP:H	2.14	0.45
1:C:726:THR:O	1:C:729:SER:HA	2.16	0.45
1:C:734:ALA:C	1:C:736:ILE:H	2.19	0.45
1:C:780:LYS:HB3	1:C:809:VAL:HG22	1.99	0.45
1:C:766:LEU:O	1:C:767:THR:C	2.56	0.45
1:A:722:VAL:HG13	1:C:852:GLU:OE1	2.16	0.45
1:A:790:GLN:O	1:A:792:PRO:HD3	2.16	0.45
1:A:794:VAL:HG12	1:A:795:GLY:N	2.32	0.45
1:A:752:ARG:CD	1:A:755:TYR:CD2	3.00	0.44
1:C:716:GLY:HA3	1:C:768:ASN:OD1	2.18	0.44
1:C:764:VAL:CG1	1:C:766:LEU:HD13	2.48	0.44
1:A:721:LYS:HE3	1:A:772:ASP:O	2.17	0.44
1:C:801:LYS:HA	1:C:861:SER:O	2.18	0.44
1:A:838:VAL:CG1	1:A:842:GLN:HE21	2.31	0.44
1:C:725:TYR:CD1	1:C:725:TYR:C	2.91	0.44
1:C:838:VAL:O	1:C:841:LYS:HG2	2.18	0.44
1:C:732:ASP:C	1:C:734:ALA:N	2.70	0.44
1:A:713:HIS:HA	1:A:714:PRO:HD3	1.82	0.44
1:C:808:GLY:O	1:C:810:TRP:CE3	2.71	0.44
1:A:780:LYS:O	1:A:781:GLU:HB2	2.17	0.44
1:C:847:LYS:HE3	1:C:859:LYS:CE	2.48	0.44
1:C:788:ASP:C	1:C:790:GLN:N	2.72	0.44
1:C:801:LYS:CA	1:C:861:SER:O	2.66	0.44
1:A:781:GLU:OE2	2:B:865:LYS:CE	2.65	0.43
1:A:766:LEU:HA	1:A:769:LEU:HD12	1.99	0.43
1:A:838:VAL:O	1:A:841:LYS:N	2.51	0.43
1:C:769:LEU:HB3	1:C:774:ILE:CD1	2.49	0.43
1:C:835:LEU:HD23	1:C:856:TRP:CG	2.53	0.43
1:C:733:LEU:HA	1:C:736:ILE:HG21	1.99	0.43
1:A:858:PHE:HZ	2:B:866:TYR:HB3	1.82	0.43
1:C:724:TYR:CE2	1:C:752:ARG:NE	2.86	0.43
1:A:831:TYR:O	1:A:832:GLU:C	2.57	0.43
1:A:733:LEU:CD1	1:A:766:LEU:HD23	2.49	0.43
1:A:719:LEU:HA	1:A:772:ASP:OD1	2.19	0.43
1:C:851:PRO:O	1:C:852:GLU:C	2.56	0.43
1:A:849:TYR:CD2	1:A:851:PRO:HG3	2.53	0.43
1:A:813:ASP:C	1:A:813:ASP:OD1	2.57	0.43
1:C:794:VAL:HA	1:C:799:ASN:OD1	2.19	0.43
1:C:737:THR:CB	1:C:743:CYS:SG	3.07	0.42
1:C:779:ARG:C	1:C:780:LYS:HG2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:ASP:OD2	1:C:816:SER:HB3	2.19	0.42
1:C:715:ALA:CB	1:C:743:CYS:CB	2.94	0.42
1:A:733:LEU:O	1:A:737:THR:CG2	2.66	0.42
1:A:848:GLU:HG3	1:A:849:TYR:N	2.33	0.42
1:C:760:PHE:CE1	1:C:802:ALA:HB2	2.54	0.42
1:C:776:HIS:HB2	1:C:783:VAL:HG12	2.01	0.42
1:C:821:LYS:O	1:C:822:SER:C	2.58	0.42
1:C:811:PRO:HG2	1:C:820:ILE:HB	2.02	0.41
1:C:750:ILE:CD1	1:C:775:VAL:HG11	2.43	0.41
1:A:838:VAL:HG12	1:A:842:GLN:HE21	1.85	0.41
1:A:808:GLY:HA2	1:A:810:TRP:CZ3	2.55	0.41
1:C:837:ALA:O	1:C:838:VAL:C	2.59	0.41
1:C:745:VAL:HG12	1:C:766:LEU:HD22	2.02	0.41
1:C:751:GLY:HA2	1:C:777:ILE:CD1	2.50	0.41
1:A:787:ASP:O	1:A:789:ASN:N	2.42	0.41
1:C:720:THR:H	1:C:772:ASP:CG	2.22	0.41
1:A:733:LEU:HD13	1:A:766:LEU:HD23	2.02	0.41
1:A:850:ARG:HB2	1:A:855:SER:HB2	2.02	0.41
1:C:784:VAL:HG21	1:C:863:PHE:CD2	2.56	0.41
2:D:869:GLN:O	2:D:870:ASP:CB	2.69	0.41
1:A:781:GLU:OE2	2:B:865:LYS:HE3	2.20	0.41
1:C:770:ASN:ND2	1:C:770:ASN:C	2.73	0.41
1:C:718:ILE:O	1:C:771:LEU:HB2	2.21	0.41
1:A:820:ILE:HG22	1:A:826:LEU:HD22	2.01	0.41
1:C:838:VAL:CG1	1:C:842:GLN:HE21	2.32	0.41
1:C:820:ILE:HG12	1:C:825:ARG:HH21	1.86	0.41
1:A:746:SER:HA	1:A:762:GLY:O	2.20	0.41
1:C:826:LEU:HD13	1:C:826:LEU:HA	1.95	0.41
1:A:744:ILE:HD12	1:A:744:ILE:N	2.36	0.41
1:A:721:LYS:HB2	1:A:724:TYR:CD2	2.56	0.40
1:A:778:ARG:NH2	1:C:803:GLU:OE2	2.53	0.40
1:C:766:LEU:HD12	1:C:769:LEU:CD1	2.52	0.40
1:C:719:LEU:HB2	1:C:771:LEU:HD12	2.02	0.40
1:A:740:LYS:HB3	1:A:742:GLU:HG3	2.04	0.40
1:A:750:ILE:O	1:A:750:ILE:HG23	2.21	0.40

All (7) 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:840:ARG:NH1	1:C:819:LEU:CG[5_655]	0.98	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ARG:NH2	1:C:819:LEU:CA[5_655]	1.50	0.70
1:A:840:ARG:NH1	1:C:819:LEU:CD2[5_655]	1.72	0.48
1:A:840:ARG:NH1	1:C:819:LEU:CB[5_655]	1.76	0.44
1:A:840:ARG:NH2	1:C:819:LEU:N[5_655]	1.78	0.42
1:A:840:ARG:CZ	1:C:819:LEU:CA[5_655]	2.13	0.07
1:A:840:ARG:CZ	1:C:819:LEU:N[5_655]	2.17	0.03

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	150/187 (80%)	124 (83%)	19 (13%)	7 (5%)	3	17
1	C	144/187 (77%)	105 (73%)	28 (19%)	11 (8%)	1	6
2	B	4/64 (6%)	3 (75%)	1 (25%)	0	100	100
2	D	4/64 (6%)	4 (100%)	0	0	100	100
All	All	302/502 (60%)	236 (78%)	48 (16%)	18 (6%)	2	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	786	LEU
1	C	714	PRO
1	C	767	THR
1	C	788	ASP
1	A	747	ASP
1	A	788	ASP
1	A	815	THR
1	C	716	GLY
1	C	731	ASP
1	C	733	LEU
1	C	743	CYS

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Mol	Chain	Res	Type
1	A	713	HIS
1	A	781	GLU
1	A	785	TYR
1	C	735	LYS
1	C	791	LYS
1	C	792	PRO
1	C	797	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	131/164 (80%)	119 (91%)	12 (9%)	11	40
1	C	129/164 (79%)	114 (88%)	15 (12%)	7	27
2	B	5/57 (9%)	4 (80%)	1 (20%)	1	8
2	D	4/57 (7%)	2 (50%)	2 (50%)	0	0
All	All	269/442 (61%)	239 (89%)	30 (11%)	7	29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	736	ILE
1	A	737	THR
1	A	738	ASN
1	A	752	ARG
1	A	766	LEU
1	A	770	ASN
1	A	775	VAL
1	A	778	ARG
1	A	787	ASP
1	A	801	LYS
1	A	826	LEU
1	A	835	LEU
2	B	868	LEU
1	C	714	PRO

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Mol	Chain	Res	Type
1	C	720	THR
1	C	738	ASN
1	C	743	CYS
1	C	747	ASP
1	C	766	LEU
1	C	770	ASN
1	C	775	VAL
1	C	778	ARG
1	C	789	ASN
1	C	801	LYS
1	C	812	THR
1	C	818	CYS
1	C	824	ASP
1	C	845	GLN
2	D	868	LEU
2	D	869	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	713	HIS
1	A	738	ASN
1	A	770	ASN
1	A	789	ASN
1	A	862	HIS
1	C	713	HIS
1	C	770	ASN

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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