Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:56 AM GMT

PDB ID	:	3CQG
Title	:	Nucleoporin Nup107/Nup133 interaction complex, delta finger mutant
Authors	:	Jeudy, S.; Boehmer, T.; Berke, I.; Schwartz, T.U.
Deposited on	:	2008-04-02
Resolution	:	3.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
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.
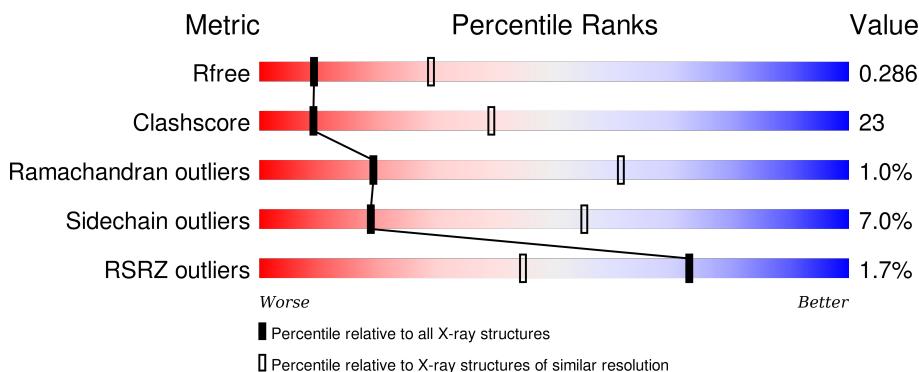
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	54% 36% • 9%
2	B	227	3% 45% 30% 6% 19%
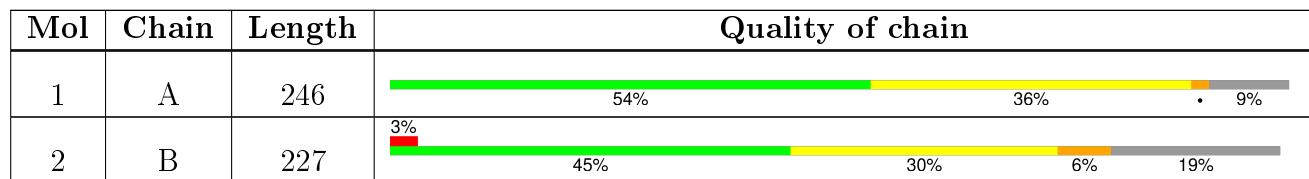
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3285 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 Nup107.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1817	1160	311	333	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	-	EXPRESSION TAG	UNP P57740
A	657	SER	-	EXPRESSION TAG	UNP P57740
A	796	GLY	-	LINKER	UNP P57740
A	797	GLY	-	LINKER	UNP P57740
A	798	SER	-	LINKER	UNP P57740
A	799	GLY	-	LINKER	UNP P57740
A	800	GLY	-	LINKER	UNP P57740
A	801	SER	-	LINKER	UNP P57740

- Molecule 2 is a protein called Nuclear pore complex protein Nup133.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1434	911	237	280	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	930	MET	-	EXPRESSION TAG	UNP Q8WUM0
B	931	ALA	-	EXPRESSION TAG	UNP Q8WUM0
B	932	SER	-	EXPRESSION TAG	UNP Q8WUM0
B	933	HIS	-	EXPRESSION TAG	UNP Q8WUM0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	5	Total 5	O 5	0	0

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.

- Molecule 1: Nuclear pore complex protein Nup107
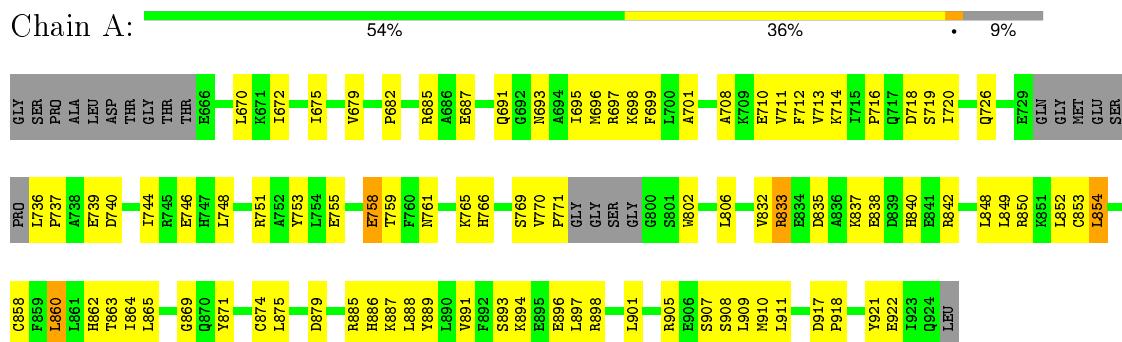
- Molecule 2: Nuclear pore complex protein Nup133
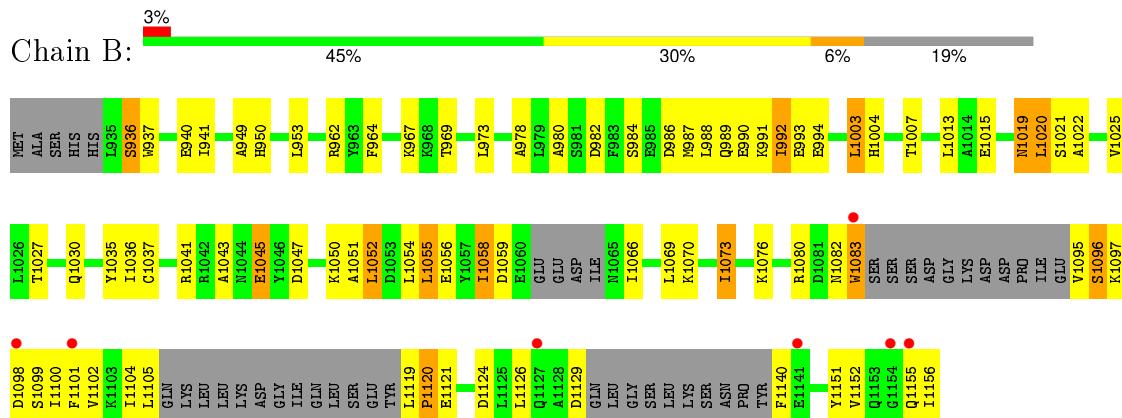
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.66Å　　65.53Å　　193.23Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	46.00　–　3.00 46.27　–　2.99	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.00-3.00) 97.4 (46.27-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$<I/\sigma(I)>$ [1]	2.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239　,　0.287 0.233　,　0.286	Depositor DCC
R_{free} test set	997 reflections (8.00%)	DCC
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	1 of 12548 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3285	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.40	0/1852	0.52	0/2495
2	B	0.35	0/1449	0.48	0/1955
All	All	0.38	0/3301	0.50	0/4450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1817	0	1797	74	0
2	B	1434	0	1397	76	0
3	A	29	0	0	1	0
3	B	5	0	0	0	0
All	All	3285	0	3194	148	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 23.

All (148) 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)
3:A:33:HOH:O	2:B:962:ARG:HG2	1.71	0.89

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1069:LEU:O	2:B:1073:ILE:HG23	1.71	0.88
2:B:1119:LEU:N	2:B:1120:PRO:CD	2.35	0.87
2:B:1097:LYS:O	2:B:1101:PHE:HD1	1.58	0.86
1:A:736:LEU:HD12	1:A:737:PRO:HD2	1.58	0.86
1:A:905:ARG:HH12	1:A:909:LEU:HD11	1.41	0.86
2:B:1126:LEU:HA	2:B:1129:ASP:OD2	1.77	0.85
2:B:1119:LEU:HD13	2:B:1155:GLN:HG2	1.56	0.84
1:A:905:ARG:NH1	1:A:909:LEU:HD11	1.94	0.82
1:A:893:SER:OG	1:A:896:GLU:HG3	1.81	0.80
1:A:720:ILE:HD13	1:A:744:ILE:HG23	1.63	0.80
1:A:771:PRO:HD2	1:A:802:TRP:NE1	2.00	0.77
1:A:739:GLU:HG2	1:A:837:LYS:HE2	1.67	0.76
2:B:936:SER:HB3	2:B:940:GLU:OE1	1.86	0.75
1:A:879:ASP:OD1	2:B:969:THR:HA	1.88	0.74
2:B:1051:ALA:HA	2:B:1054:LEU:HD12	1.70	0.74
2:B:1126:LEU:O	2:B:1129:ASP:HB2	1.87	0.73
2:B:1083:TRP:HA	2:B:1083:TRP:CE3	2.25	0.72
1:A:833:ARG:CG	1:A:833:ARG:HH11	2.04	0.71
1:A:849:LEU:HD23	1:A:852:LEU:HD12	1.73	0.70
2:B:1119:LEU:N	2:B:1120:PRO:HD2	2.05	0.70
2:B:1036:ILE:CG2	2:B:1076:LYS:HD2	2.21	0.69
2:B:1043:ALA:HB3	2:B:1080:ARG:HH12	1.58	0.68
2:B:1097:LYS:O	2:B:1101:PHE:CD1	2.46	0.66
2:B:1083:TRP:HA	2:B:1083:TRP:HE3	1.59	0.66
1:A:848:LEU:O	1:A:852:LEU:HG	1.95	0.66
2:B:1043:ALA:HB3	2:B:1080:ARG:NH1	2.10	0.65
2:B:1101:PHE:O	2:B:1104:ILE:HG12	1.97	0.65
1:A:850:ARG:O	1:A:854:LEU:HB2	1.97	0.64
2:B:1100:ILE:O	2:B:1104:ILE:HG23	1.98	0.62
2:B:1083:TRP:HH2	2:B:1095:VAL:N	1.96	0.62
1:A:769:SER:C	1:A:771:PRO:HD3	2.19	0.62
1:A:875:LEU:HD21	1:A:908:SER:OG	1.99	0.62
1:A:771:PRO:HD2	1:A:802:TRP:HE1	1.65	0.60
1:A:758:GLU:HG2	1:A:759:THR:N	2.15	0.60
2:B:989:GLN:O	2:B:993:GLU:HB2	2.03	0.58
1:A:687:GLU:O	1:A:691:GLN:HG3	2.02	0.58
1:A:675:ILE:O	1:A:679:VAL:HG23	2.03	0.58
1:A:736:LEU:O	1:A:833:ARG:NH2	2.37	0.58
1:A:770:VAL:N	1:A:771:PRO:HD3	2.19	0.58
2:B:1045:GLU:HG2	2:B:1099:SER:OG	2.03	0.57
2:B:1126:LEU:HA	2:B:1129:ASP:CG	2.25	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:LEU:HB3	2:B:980:ALA:HB2	1.87	0.57
2:B:1083:TRP:CH2	2:B:1095:VAL:N	2.73	0.57
1:A:894:LYS:O	1:A:898:ARG:HG3	2.05	0.56
1:A:833:ARG:NH1	1:A:833:ARG:CG	2.66	0.56
2:B:1119:LEU:N	2:B:1120:PRO:HD3	2.21	0.56
2:B:1019:ASN:CB	2:B:1022:ALA:HB3	2.36	0.56
1:A:833:ARG:NH1	1:A:833:ARG:HG2	2.20	0.56
1:A:833:ARG:HG3	1:A:835:ASP:OD1	2.05	0.56
2:B:1097:LYS:O	2:B:1100:ILE:HG12	2.07	0.55
1:A:875:LEU:HD21	1:A:908:SER:HG	1.71	0.54
2:B:1140:PHE:CG	2:B:1140:PHE:O	2.60	0.53
1:A:701:ALA:HA	1:A:852:LEU:HD13	1.90	0.53
2:B:1015:GLU:OE1	2:B:1041:ARG:NH2	2.42	0.53
1:A:869:GLY:HA2	1:A:871:TYR:CE1	2.44	0.53
2:B:1095:VAL:O	2:B:1098:ASP:HB2	2.08	0.53
1:A:736:LEU:HD12	1:A:737:PRO:CD	2.36	0.53
2:B:1019:ASN:O	2:B:1021:SER:N	2.42	0.53
2:B:1104:ILE:HD11	2:B:1119:LEU:HD21	1.90	0.52
1:A:833:ARG:HG2	1:A:833:ARG:HH11	1.73	0.52
2:B:1052:LEU:HD13	2:B:1073:ILE:HG12	1.92	0.52
2:B:984:SER:HB3	2:B:987:MET:HB2	1.91	0.52
2:B:953:LEU:HD13	2:B:973:LEU:HB3	1.92	0.52
1:A:865:LEU:HB2	1:A:874:CYS:SG	2.50	0.52
1:A:888:LEU:O	1:A:891:VAL:HG22	2.10	0.51
1:A:696:MET:HE3	1:A:712:PHE:HB2	1.91	0.51
1:A:917:ASP:HB2	1:A:918:PRO:CD	2.40	0.51
2:B:1051:ALA:O	2:B:1054:LEU:HB2	2.11	0.51
2:B:1043:ALA:HA	2:B:1047:ASP:OD2	2.10	0.51
1:A:740:ASP:O	1:A:744:ILE:HG13	2.10	0.51
2:B:967:LYS:HD2	2:B:1025:VAL:HG21	1.93	0.51
1:A:917:ASP:OD2	1:A:921:TYR:HB2	2.11	0.51
1:A:699:PHE:HD2	1:A:708:ALA:HA	1.76	0.51
2:B:1052:LEU:HD22	2:B:1073:ILE:HD11	1.93	0.50
2:B:1152:VAL:O	2:B:1156:ILE:HG12	2.11	0.50
2:B:937:TRP:O	2:B:941:ILE:HG13	2.11	0.50
1:A:682:PRO:O	1:A:726:GLN:NE2	2.45	0.50
2:B:1015:GLU:OE2	2:B:1041:ARG:NH2	2.43	0.50
1:A:832:VAL:O	1:A:832:VAL:HG12	2.10	0.50
2:B:1027:THR:OG1	2:B:1030:GLN:HG3	2.11	0.50
2:B:990:GLU:O	2:B:993:GLU:HB3	2.12	0.49
2:B:964:PHE:HA	2:B:1025:VAL:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:TYR:CZ	1:A:910:MET:HG2	2.47	0.49
2:B:1036:ILE:HG22	2:B:1076:LYS:HD2	1.92	0.49
1:A:871:TYR:HB2	1:A:911:LEU:HD21	1.93	0.49
1:A:685:ARG:HD2	1:A:719:SER:HB3	1.94	0.48
2:B:1070:LYS:HZ2	2:B:1121:GLU:HB2	1.78	0.48
2:B:1102:VAL:O	2:B:1105:LEU:HG	2.12	0.48
2:B:1151:TYR:O	2:B:1155:GLN:HG3	2.12	0.48
1:A:854:LEU:HA	1:A:854:LEU:HD12	1.64	0.48
2:B:1003:LEU:O	2:B:1007:THR:HG23	2.13	0.48
2:B:1152:VAL:O	2:B:1156:ILE:HG23	2.14	0.48
2:B:989:GLN:HA	2:B:992:ILE:HG23	1.97	0.47
2:B:1052:LEU:HD12	2:B:1055:LEU:HD23	1.97	0.46
1:A:755:GLU:O	1:A:759:THR:HG23	2.15	0.46
2:B:1082:ASN:O	2:B:1083:TRP:C	2.53	0.46
1:A:687:GLU:HG3	1:A:691:GLN:HE21	1.81	0.46
2:B:1019:ASN:HD22	2:B:1022:ALA:HB3	1.81	0.46
2:B:1119:LEU:HB3	2:B:1155:GLN:CD	2.37	0.45
1:A:761:ASN:O	1:A:765:LYS:HG2	2.16	0.45
1:A:887:LYS:HA	1:A:889:TYR:CE1	2.52	0.45
1:A:897:LEU:O	1:A:901:LEU:HG	2.17	0.45
2:B:949:ALA:O	2:B:953:LEU:HB2	2.16	0.45
2:B:988:LEU:O	2:B:992:ILE:HG22	2.17	0.44
2:B:1019:ASN:O	2:B:1020:LEU:C	2.56	0.44
1:A:885:ARG:HB2	1:A:886:HIS:CD2	2.53	0.44
2:B:1020:LEU:HD23	2:B:1021:SER:H	1.82	0.44
2:B:984:SER:HB3	2:B:987:MET:CB	2.47	0.44
1:A:893:SER:HG	1:A:896:GLU:HG3	1.81	0.44
2:B:1058:ILE:CG2	2:B:1059:ASP:N	2.81	0.44
1:A:710:GLU:O	1:A:713:VAL:HG22	2.18	0.44
2:B:1041:ARG:C	2:B:1043:ALA:H	2.21	0.43
1:A:838:GLU:OE1	1:A:840:HIS:CE1	2.71	0.43
1:A:718:ASP:OD1	1:A:718:ASP:C	2.56	0.43
1:A:670:LEU:C	1:A:670:LEU:HD23	2.38	0.43
1:A:679:VAL:O	1:A:679:VAL:HG12	2.17	0.43
1:A:712:PHE:CZ	1:A:751:ARG:HG3	2.53	0.43
1:A:862:HIS:HE1	1:A:907:SER:OG	2.01	0.43
1:A:693:ASN:HB3	1:A:746:GLU:OE2	2.18	0.43
1:A:832:VAL:CG1	1:A:832:VAL:O	2.66	0.43
1:A:697:ARG:CZ	1:A:842:ARG:HG3	2.49	0.42
1:A:695:ILE:O	1:A:698:LYS:HB3	2.19	0.42
1:A:875:LEU:HD12	1:A:875:LEU:N	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1124:ASP:C	2:B:1124:ASP:OD1	2.58	0.42
2:B:1035:TYR:CZ	2:B:1050:LYS:HD2	2.54	0.42
2:B:1050:LYS:O	2:B:1054:LEU:HG	2.19	0.42
2:B:1045:GLU:H	2:B:1045:GLU:HG3	1.53	0.42
2:B:950:HIS:ND1	2:B:978:ALA:HB2	2.35	0.42
1:A:753:TYR:CE1	1:A:853:CYS:HB3	2.54	0.42
1:A:863:THR:O	1:A:864:ILE:C	2.57	0.41
1:A:850:ARG:HA	1:A:854:LEU:HD22	2.02	0.41
2:B:1019:ASN:HB3	2:B:1022:ALA:HB3	2.02	0.41
2:B:1015:GLU:CD	2:B:1041:ARG:NH2	2.74	0.41
1:A:711:VAL:HA	1:A:714:LYS:HD2	2.02	0.41
2:B:1104:ILE:O	2:B:1105:LEU:C	2.59	0.41
2:B:1058:ILE:HG22	2:B:1059:ASP:N	2.36	0.41
1:A:748:LEU:HD23	1:A:748:LEU:HA	1.88	0.41
2:B:1004:HIS:CG	2:B:1054:LEU:HD21	2.54	0.41
2:B:1096:SER:HA	2:B:1099:SER:OG	2.21	0.41
1:A:897:LEU:HA	1:A:897:LEU:HD23	1.96	0.41
1:A:766:HIS:HD2	1:A:806:LEU:HD13	1.86	0.40
1:A:833:ARG:HH11	1:A:833:ARG:HG3	1.80	0.40
1:A:691:GLN:O	1:A:695:ILE:HG13	2.21	0.40
1:A:860:LEU:HD12	1:A:860:LEU:HA	1.77	0.40
2:B:1058:ILE:HG21	2:B:1066:ILE:HD11	2.03	0.40
1:A:720:ILE:CD1	1:A:744:ILE:HG23	2.42	0.40
1:A:696:MET:HE1	1:A:712:PHE:HD1	1.86	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	219/246 (89%)	203 (93%)	15 (7%)	1 (0%)	34	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/227 (77%)	155 (89%)	16 (9%)	3 (2%)	11	46
All	All	393/473 (83%)	358 (91%)	31 (8%)	4 (1%)	19	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1020	LEU
1	A	716	PRO
2	B	1019	ASN
2	B	1120	PRO

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	195/215 (91%)	188 (96%)	7 (4%)	42	79
2	B	149/203 (73%)	132 (89%)	17 (11%)	7	28
All	All	344/418 (82%)	320 (93%)	24 (7%)	19	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	672	ILE
1	A	758	GLU
1	A	833	ARG
1	A	854	LEU
1	A	858	CYS
1	A	860	LEU
1	A	922	GLU
2	B	936	SER
2	B	982	ASP
2	B	986	ASP
2	B	991	LYS
2	B	992	ILE

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
2	B	994	GLU
2	B	1003	LEU
2	B	1013	LEU
2	B	1037	CYS
2	B	1045	GLU
2	B	1052	LEU
2	B	1055	LEU
2	B	1056	GLU
2	B	1058	ILE
2	B	1073	ILE
2	B	1083	TRP
2	B	1096	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	691	GLN
1	A	766	HIS
1	A	840	HIS
1	A	844	HIS
1	A	862	HIS
1	A	886	HIS
1	A	914	GLN
2	B	958	ASN
2	B	1019	ASN
2	B	1147	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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	225/246 (91%)	-0.24	0 100	100	44, 64, 92, 116	0
2	B	184/227 (81%)	0.03	7 (3%) 44	18	55, 89, 181, 193	0
All	All	409/473 (86%)	-0.12	7 (1%) 73	45	44, 73, 140, 193	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1083	TRP	4.7
2	B	1155	GLN	3.9
2	B	1127	GLN	3.2
2	B	1154	GLY	3.2
2	B	1101	PHE	2.3
2	B	1098	ASP	2.1
2	B	1141	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.