



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2016 – 03:29 PM EDT

PDB ID : 5ICA  
Title : Structure of the CTD complex of UTP12, Utp13, Utp1 and Utp21  
Authors : Zhang, C.; Ye, K.  
Deposited on : 2016-02-23  
Resolution : 3.51 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

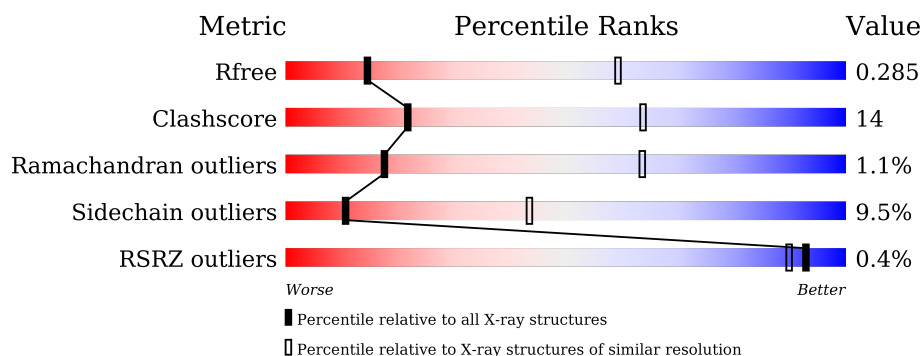
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	163	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 34%, orange 6%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>61%</span> <span>34%</span> <span>6%</span> </div> </div>
2	B	152	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 55%, yellow 31%, orange 5%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>55%</span> <span>31%</span> <span>5%</span> <span>9%</span> </div> </div>
3	C	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 40%, yellow 10%, grey 48%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span></span> <span>40%</span> <span>10%</span> <span>48%</span> </div> </div>
4	D	149	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 51%, yellow 26%, orange 1%, grey 20%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span></span> <span>51%</span> <span>26%</span> <span>20%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4377 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1293	827	232	228	6			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	0	0	0
			1116	711	197	208			

- Molecule 3 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	128	Total	C	N	O	S	0	0	0
			997	632	176	186	3			

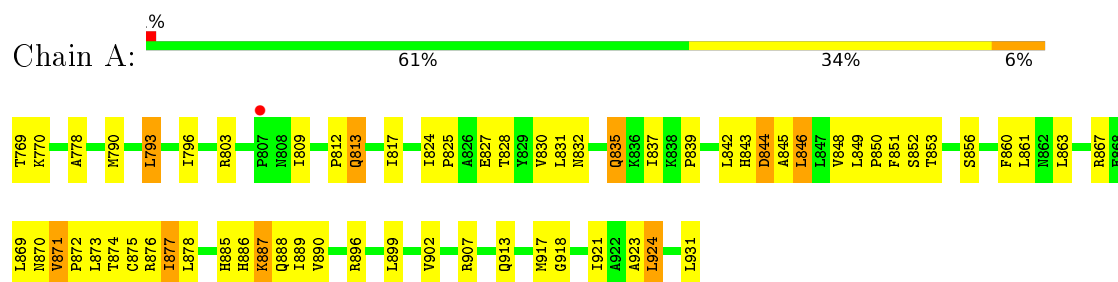
- Molecule 4 is a protein called Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			971	628	171	167	5			

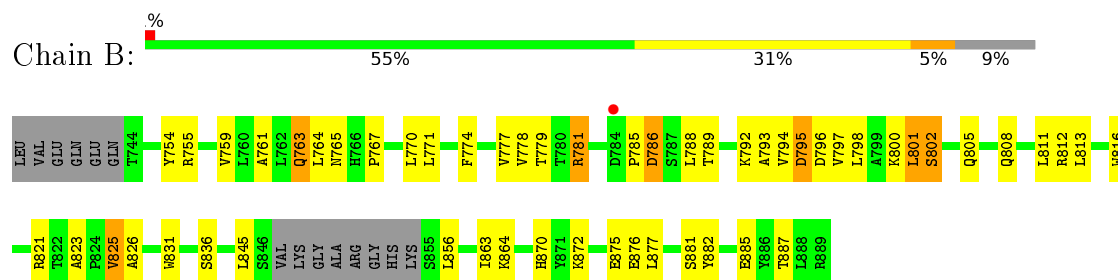
### 3 Residue-property plots

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.

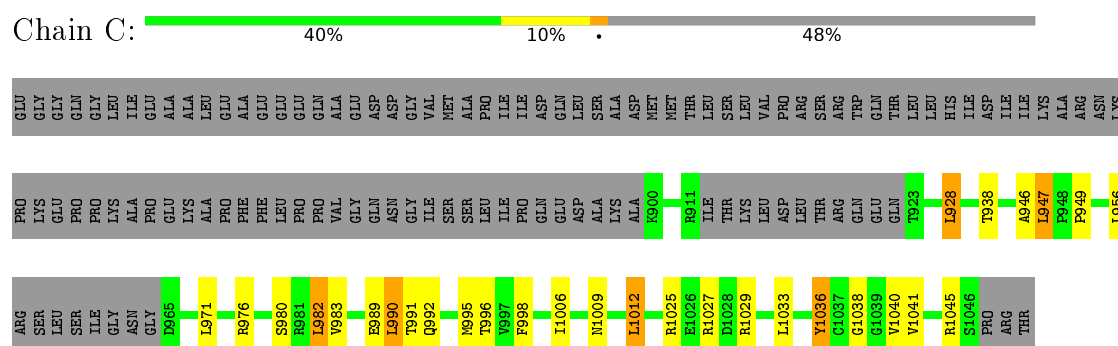
- Molecule 1: Putative uncharacterized protein



- Molecule 2: Putative uncharacterized protein



- Molecule 3: Putative U3 snoRNP protein



- Molecule 4: Periodic tryptophan protein 2-like protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.69Å 121.69Å 167.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.38 – 3.51 34.38 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.38-3.51) 85.2 (34.38-3.51)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.244 , 0.275 0.249 , 0.285	Depositor DCC
$R_{free}$ test set	1611 reflections (9.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.2	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.39	0/1314	0.56	0/1782
2	B	0.40	0/1136	0.54	0/1546
3	C	0.35	0/1013	0.53	2/1368 (0.1%)
4	D	0.35	0/991	0.55	0/1346
All	All	0.38	0/4454	0.55	2/6042 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	928	LEU	CA-CB-CG	5.87	128.79	115.30
3	C	947	LEU	CA-CB-CG	5.53	128.01	115.30

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	1293	0	1365	44	0
2	B	1116	0	1130	44	0
3	C	997	0	962	21	0
4	D	971	0	995	32	0
All	All	4377	0	4452	124	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 14.

All (124) 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:917:MET:HE1	2:B:870:HIS:HB2	1.63	0.79
4:D:782:GLU:OE2	4:D:821:ARG:NH1	2.22	0.71
2:B:778:VAL:HG21	2:B:825:VAL:HG12	1.72	0.71
4:D:741:ASN:OD1	4:D:772:ARG:NH2	2.27	0.68
1:A:861:LEU:HD11	1:A:877:ILE:HD11	1.75	0.68
4:D:809:ARG:HE	4:D:810:GLY:H	1.41	0.68
1:A:924:LEU:HD11	2:B:863:ILE:HG22	1.77	0.65
1:A:827:GLU:HG2	1:A:863:LEU:HD23	1.78	0.65
4:D:827:ARG:NH1	4:D:828:ASP:OD1	2.31	0.63
3:C:1027:ARG:HE	4:D:835:ASP:HB3	1.63	0.63
3:C:1009:ASN:HB3	3:C:1012:LEU:HD11	1.80	0.62
4:D:835:ASP:HA	4:D:838:VAL:HG12	1.81	0.62
2:B:755:ARG:HD2	2:B:800:LYS:NZ	2.14	0.61
3:C:982:LEU:HD22	3:C:991:THR:HG21	1.82	0.61
1:A:825:PRO:O	1:A:828:THR:HG22	2.01	0.60
1:A:844:ASP:OD1	1:A:844:ASP:N	2.34	0.59
3:C:1033:LEU:HD21	4:D:792:LEU:HD12	1.84	0.58
1:A:887:LYS:H	1:A:887:LYS:HD3	1.70	0.56
3:C:971:LEU:HD22	3:C:998:PHE:HE1	1.70	0.56
2:B:785:PRO:HG2	2:B:792:LYS:HG3	1.88	0.56
1:A:913:GLN:O	1:A:917:MET:HG3	2.06	0.55
4:D:730:TYR:CD1	4:D:753:ILE:HG22	2.41	0.55
2:B:786:ASP:N	2:B:786:ASP:OD1	2.39	0.55
2:B:761:ALA:HB1	2:B:770:LEU:HB2	1.90	0.54
1:A:907:ARG:NH1	2:B:885:GLU:OE2	2.40	0.54
2:B:778:VAL:HG23	2:B:779:THR:HG23	1.88	0.54
4:D:755:TYR:CE1	4:D:756:THR:HG23	2.42	0.54
1:A:861:LEU:HD21	1:A:877:ILE:HD11	1.89	0.54
2:B:882:TYR:HD1	2:B:885:GLU:HG3	1.74	0.53
4:D:758:ILE:HD13	4:D:793:TRP:CD1	2.44	0.53
1:A:867:ARG:HD2	2:B:781:ARG:HD2	1.91	0.53
2:B:875:GLU:OE2	4:D:832:ARG:NH1	2.42	0.53
3:C:1029:ARG:HD3	4:D:788:GLU:OE2	2.09	0.53
3:C:1038:GLY:HA2	4:D:823:VAL:HG21	1.91	0.53
2:B:798:LEU:HA	2:B:801:LEU:HD23	1.91	0.52
2:B:755:ARG:HD2	2:B:800:LYS:HZ3	1.75	0.51
4:D:775:ARG:HG3	4:D:815:GLU:HG3	1.92	0.51
1:A:918:GLY:O	1:A:921:ILE:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:781:THR:HG23	4:D:826:MET:HE2	1.92	0.51
3:C:1036:TYR:O	3:C:1040:VAL:HG23	2.11	0.51
1:A:870:ASN:O	1:A:874:THR:HG22	2.10	0.51
1:A:828:THR:O	1:A:832:ASN:ND2	2.44	0.50
1:A:924:LEU:HD13	2:B:864:LYS:HA	1.93	0.49
1:A:885:HIS:O	1:A:889:ILE:HG12	2.13	0.49
1:A:873:LEU:O	1:A:877:ILE:HG23	2.12	0.49
1:A:778:ALA:HB1	1:A:837:ILE:HD13	1.94	0.48
2:B:755:ARG:O	2:B:759:VAL:HG23	2.13	0.48
3:C:1041:VAL:O	3:C:1045:ARG:HG3	2.14	0.48
2:B:798:LEU:O	2:B:801:LEU:HB2	2.14	0.48
3:C:976:ARG:HA	3:C:976:ARG:HD2	1.76	0.48
1:A:793:LEU:O	1:A:796:ILE:HG13	2.14	0.47
3:C:989:GLU:HG2	3:C:990:LEU:N	2.29	0.47
4:D:815:GLU:O	4:D:818:VAL:HG12	2.14	0.47
2:B:755:ARG:HG2	2:B:797:VAL:HG23	1.95	0.47
2:B:774:PHE:O	2:B:778:VAL:HG13	2.15	0.47
2:B:788:LEU:HB2	2:B:795:ASP:OD2	2.14	0.47
1:A:835:GLN:OE1	2:B:821:ARG:NH1	2.47	0.47
4:D:758:ILE:O	4:D:762:VAL:HG23	2.15	0.47
2:B:795:ASP:N	2:B:795:ASP:OD1	2.46	0.47
1:A:831:LEU:O	1:A:835:GLN:HG3	2.14	0.47
1:A:871:VAL:HG23	1:A:872:PRO:HD3	1.97	0.47
1:A:875:CYS:O	1:A:878:LEU:N	2.48	0.46
1:A:812:PRO:O	1:A:813:GLN:HG3	2.16	0.46
1:A:931:LEU:HD21	2:B:856:LEU:HD23	1.97	0.46
2:B:882:TYR:HA	2:B:885:GLU:HG2	1.96	0.46
4:D:788:GLU:O	4:D:792:LEU:HB2	2.15	0.46
3:C:989:GLU:HG2	3:C:990:LEU:HD22	1.98	0.46
4:D:745:LEU:HD13	4:D:745:LEU:HA	1.78	0.46
3:C:1045:ARG:NH2	4:D:817:ARG:HG3	2.30	0.46
2:B:796:ASP:O	2:B:800:LYS:HG3	2.16	0.46
2:B:808:GLN:HB3	2:B:812:ARG:HH22	1.81	0.46
4:D:823:VAL:O	4:D:827:ARG:N	2.48	0.45
1:A:887:LYS:HA	1:A:890:VAL:HG22	1.98	0.45
1:A:850:PRO:O	1:A:853:THR:OG1	2.32	0.45
1:A:851:PHE:CE1	1:A:888:GLN:HB3	2.52	0.45
1:A:924:LEU:HD22	2:B:864:LYS:HB2	1.99	0.45
3:C:980:SER:O	3:C:983:VAL:HG12	2.16	0.45
1:A:830:VAL:HG21	1:A:860:PHE:CE1	2.52	0.45
1:A:845:ALA:O	1:A:848:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1036:TYR:CE1	3:C:1040:VAL:HG21	2.52	0.45
2:B:802:SER:OG	2:B:805:GLN:HG3	2.17	0.45
4:D:758:ILE:HD13	4:D:793:TRP:NE1	2.32	0.45
4:D:774:LEU:HD23	4:D:797:LEU:HD13	1.99	0.45
1:A:923:ALA:HA	4:D:843:TYR:CE2	2.52	0.45
3:C:1006:ILE:HD11	4:D:844:LEU:HD13	1.98	0.44
4:D:827:ARG:HG3	4:D:831:ARG:HD2	1.99	0.44
2:B:788:LEU:HA	2:B:831:TRP:HZ3	1.82	0.44
1:A:849:LEU:HD22	1:A:853:THR:OG1	2.18	0.44
2:B:771:LEU:HB2	2:B:816:TRP:CZ2	2.52	0.44
4:D:787:MET:HG2	4:D:826:MET:SD	2.58	0.44
1:A:827:GLU:HG3	1:A:827:GLU:H	1.57	0.43
4:D:773:LEU:O	4:D:777:VAL:HG22	2.18	0.43
4:D:794:ILE:HD13	4:D:819:VAL:HG13	2.00	0.43
1:A:842:LEU:HD23	1:A:876:ARG:HE	1.83	0.43
1:A:790:MET:HG2	1:A:856:SER:OG	2.18	0.43
3:C:1027:ARG:NE	4:D:835:ASP:HB3	2.33	0.43
2:B:754:TYR:CZ	2:B:793:ALA:HB1	2.54	0.42
1:A:846:LEU:HA	1:A:846:LEU:HD13	1.77	0.42
2:B:764:LEU:HA	2:B:764:LEU:HD23	1.84	0.42
3:C:1006:ILE:HB	3:C:1012:LEU:HD13	2.00	0.42
1:A:831:LEU:HD22	1:A:869:LEU:HB3	2.02	0.42
1:A:839:PRO:O	1:A:842:LEU:HB3	2.19	0.42
1:A:830:VAL:HG21	1:A:860:PHE:CZ	2.55	0.42
2:B:765:ASN:HA	2:B:812:ARG:HH11	1.83	0.42
2:B:763:GLN:OE1	2:B:805:GLN:NE2	2.53	0.42
2:B:789:THR:HG21	2:B:794:VAL:HG11	2.02	0.42
3:C:992:GLN:O	3:C:996:THR:HG22	2.20	0.42
1:A:899:LEU:HA	1:A:902:VAL:HG12	2.01	0.42
2:B:877:LEU:O	2:B:881:SER:HB3	2.20	0.42
4:D:762:VAL:HG11	4:D:797:LEU:HA	2.01	0.42
2:B:882:TYR:CD1	2:B:885:GLU:HG3	2.54	0.41
4:D:815:GLU:O	4:D:819:VAL:HG23	2.21	0.41
1:A:887:LYS:HG2	1:A:888:GLN:OE1	2.19	0.41
2:B:823:ALA:O	2:B:826:ALA:HB3	2.21	0.41
2:B:813:LEU:HD23	2:B:813:LEU:HA	1.76	0.41
3:C:989:GLU:HG2	3:C:990:LEU:HD13	2.02	0.41
1:A:824:ILE:HD12	1:A:828:THR:HG23	2.03	0.41
2:B:813:LEU:HD23	2:B:816:TRP:HE3	1.86	0.41
2:B:808:GLN:HB3	2:B:812:ARG:NH2	2.36	0.41
2:B:778:VAL:HG12	2:B:789:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:LEU:HD23	1:A:850:PRO:HD2	2.03	0.40
2:B:872:LYS:O	2:B:876:GLU:HG3	2.21	0.40
2:B:774:PHE:O	2:B:777:VAL:HG12	2.22	0.40
3:C:1025:ARG:HD3	3:C:1025:ARG:HA	1.76	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	161/163 (99%)	146 (91%)	12 (8%)	3 (2%)	10	51
2	B	134/152 (88%)	128 (96%)	6 (4%)	0	100	100
3	C	122/244 (50%)	109 (89%)	11 (9%)	2 (2%)	12	55
4	D	117/149 (78%)	104 (89%)	12 (10%)	1 (1%)	21	68
All	All	534/708 (75%)	487 (91%)	41 (8%)	6 (1%)	17	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	886	HIS
1	A	809	ILE
1	A	835	GLN
3	C	946	ALA
4	D	834	ALA
3	C	949	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	142/142 (100%)	127 (89%)	15 (11%)	8	38
2	B	123/134 (92%)	111 (90%)	12 (10%)	10	42
3	C	98/202 (48%)	89 (91%)	9 (9%)	11	45
4	D	102/129 (79%)	94 (92%)	8 (8%)	16	53
All	All	465/607 (77%)	421 (90%)	44 (10%)	11	43

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	769	THR
1	A	770	LYS
1	A	793	LEU
1	A	803	ARG
1	A	813	GLN
1	A	817	ILE
1	A	843	HIS
1	A	844	ASP
1	A	846	LEU
1	A	852	SER
1	A	871	VAL
1	A	877	ILE
1	A	887	LYS
1	A	896	ARG
1	A	924	LEU
2	B	763	GLN
2	B	767	PRO
2	B	781	ARG
2	B	786	ASP
2	B	795	ASP
2	B	801	LEU
2	B	802	SER
2	B	811	LEU
2	B	825	VAL
2	B	836	SER
2	B	845	LEU
2	B	887	THR
3	C	928	LEU

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Mol	Chain	Res	Type
3	C	938	THR
3	C	947	LEU
3	C	956	LEU
3	C	982	LEU
3	C	990	LEU
3	C	995	MET
3	C	1012	LEU
3	C	1036	TYR
4	D	740	LEU
4	D	755	TYR
4	D	777	VAL
4	D	792	LEU
4	D	799	ASP
4	D	812	VAL
4	D	815	GLU
4	D	830	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	163/163 (100%)	-0.37	1 (0%) 90 85	61, 92, 142, 169	0
2	B	138/152 (90%)	-0.40	1 (0%) 89 82	76, 111, 144, 155	0
3	C	128/244 (52%)	-0.23	0 100 100	82, 133, 157, 166	0
4	D	119/149 (79%)	-0.44	0 100 100	72, 98, 127, 139	0
All	All	548/708 (77%)	-0.36	2 (0%) 93 90	61, 107, 149, 169	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	807	PRO	2.7
2	B	784	ASP	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.