



Full wwPDB X-ray Structure Validation Report

May 15, 2020 – 04:45 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

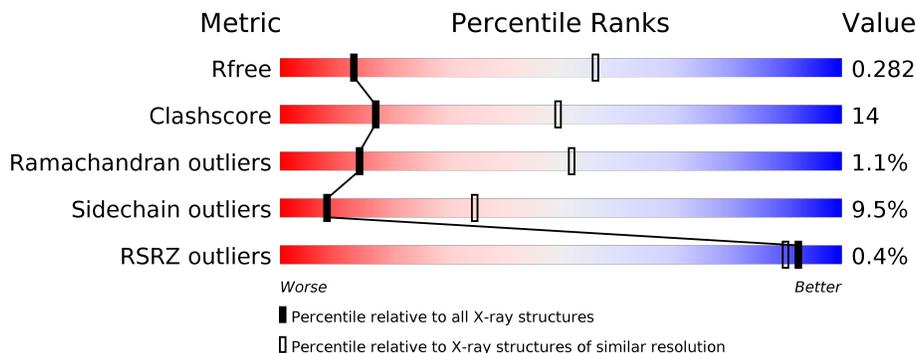
1 Overall quality at a glance

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 % 61% 34% 6%
2	B	152	 % 55% 31% 5% 9%
3	C	244	 40% 10% 48%
4	D	149	 51% 26% 20%

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
			Total	C	N	O	S			
1	A	163	1293	827	232	228	6	0	0	0

- Molecule 2 is a protein called Putative uncharacterized protein.

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

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

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

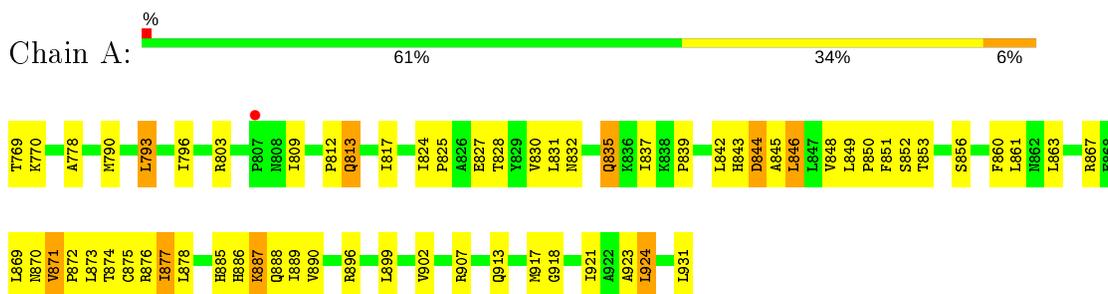
- Molecule 4 is a protein called Periodic tryptophan protein 2-like protein.

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

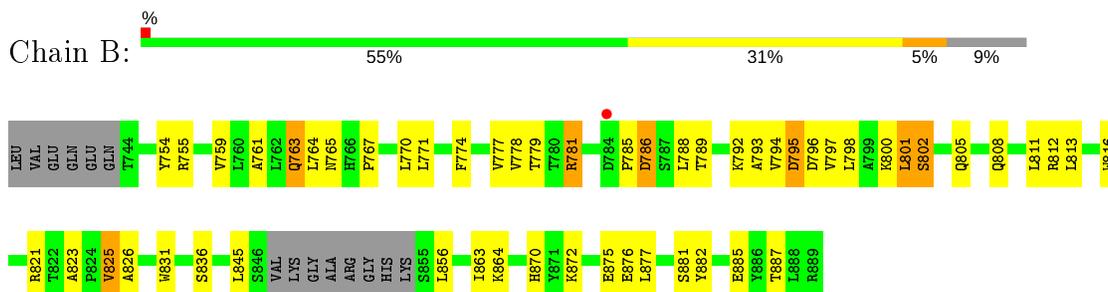
3 Residue-property plots [i](#)

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

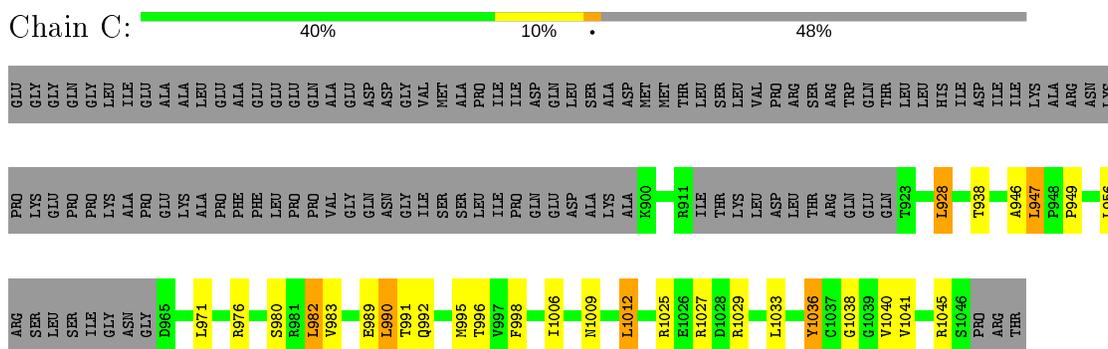
- Molecule 1: Putative uncharacterized protein



- Molecule 2: Putative uncharacterized protein



- Molecule 3: Putative U3 snoRNP protein



- Molecule 4: Periodic tryptophan protein 2-like protein



ASP	ASP
ASN	THR
THR	VAL
VAL	GLN
GLN	PHE
PHE	ASP
ASP	PRO
PRO	PHE
PHE	ASP
ASP	LEU
LEU	ASN
ASN	MET
MET	GLU
GLU	ILE
ILE	THR
THR	PRO
PRO	ALA
ALA	SER
SER	THR
THR	LEU
LEU	ALA
ALA	VAL
VAL	LEU
LEU	GLU
GLU	LYS
LYS	GLU
GLU	LYS
LYS	Y729
Y729	Y730
Y730	L740
L740	M741
M741	L745
L745	I753
I753	F754
F754	Y755
Y755	T756
T756	D757
D757	I758
I758	V762
V762	R772
R772	L773
L773	L774
L774	R775
R775	F776
F776	V777
V777	T781
T781	E782
E782	M787
M787	E788
E788	L792
L792	M793
M793	I794
I794	L797
L797	I798
I798	D799
D799	R809
R809	G810
G810	R811
R811	V812
V812	E815
E815	L816
L816	R817
R817	V818
V818	V819
V819	A820
A820	R821
R821	A822
A822	V823
V823	M826
M826	R827
R827	D828
D828	E829
E829	I830
I830	R831
R831	R832
R832	L833
L833	A834
A834	D835
D835	V838
V838	Y843
Y843	L844
L844	Q847
Q847	ALA
ALA	LYS
LYS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.47Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.275 0.255 , 0.282	Depositor DCC
R_{free} test set	1832 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4377	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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($^{\circ}$)	Ideal($^{\circ}$)
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:845:ALA:O	1:A:848:VAL:HG12	2.17	0.45
1:A:830:VAL:HG21	1:A:860:PHE:CE1	2.52	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
1:A:923:ALA:HA	4:D:843:TYR:CE2	2.52	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
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%)	8	40
2	B	134/152 (88%)	128 (96%)	6 (4%)	0	100	100
3	C	122/244 (50%)	109 (89%)	11 (9%)	2 (2%)	9	43
4	D	117/149 (78%)	104 (89%)	12 (10%)	1 (1%)	17	56
All	All	534/708 (75%)	487 (91%)	41 (8%)	6 (1%)	14	52

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%)	6	30
2	B	123/134 (92%)	111 (90%)	12 (10%)	8	33
3	C	98/202 (48%)	89 (91%)	9 (9%)	9	36
4	D	102/129 (79%)	94 (92%)	8 (8%)	12	42
All	All	465/607 (77%)	421 (90%)	44 (10%)	8	34

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, 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	163/163 (100%)	-0.38	1 (0%) 89 86	61, 92, 142, 169	0
2	B	138/152 (90%)	-0.41	1 (0%) 87 83	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%) 92 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.