Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 08:03 AM EDT

PDB ID	:	8U4U
Title	:	Crystal structure of 53BP1 tandem Tudor domain homodimer engineered with two disulfide bridges
Authors	:	Cui, G.; Botuyan, M.V.; Thompson, J.R.; Mer, G.
Deposited on	:	2023-09-11
Resolution	:	3.79 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

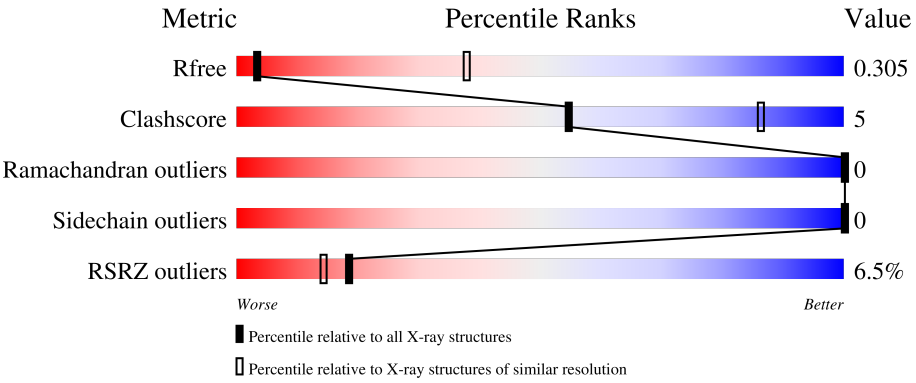
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 of 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 <=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	125	3% 80% 15% 5%
1	B	125	4% 81% 14% 5%
1	C	125	6% 84% 11% 5%
1	D	125	10% 82% 13% 5%
1	E	125	7% 87% 8% 5%

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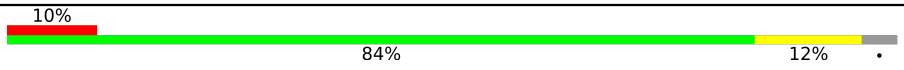
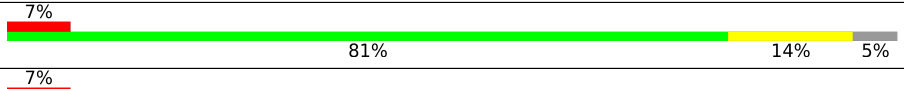
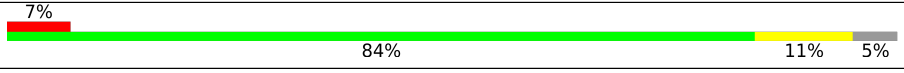
Mol	Chain	Length	Quality of chain
1	F	125	
1	G	125	
1	H	125	
1	I	125	
1	J	125	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18847 atoms, of which 9357 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 TP53-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	119	Total	C	H	N	O	S	0	0	0
			1885	606	936	160	178	5			
1	B	119	Total	C	H	N	O	S	0	0	0
			1877	604	932	159	177	5			
1	C	119	Total	C	H	N	O	S	0	0	0
			1877	604	932	159	177	5			
1	D	119	Total	C	H	N	O	S	0	0	0
			1877	604	932	159	177	5			
1	E	119	Total	C	H	N	O	S	0	0	0
			1885	606	936	160	178	5			
1	F	120	Total	C	H	N	O	S	0	0	0
			1892	608	939	161	179	5			
1	G	120	Total	C	H	N	O	S	0	0	0
			1892	608	939	161	179	5			
1	H	120	Total	C	H	N	O	S	0	0	0
			1892	608	939	161	179	5			
1	I	119	Total	C	H	N	O	S	0	0	0
			1885	606	936	160	178	5			
1	J	119	Total	C	H	N	O	S	0	0	0
			1885	606	936	160	178	5			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1479	GLY	-	expression tag	UNP Q12888
A	1480	PRO	-	expression tag	UNP Q12888
A	1481	GLY	-	expression tag	UNP Q12888
A	1482	HIS	-	expression tag	UNP Q12888
A	1483	MET	-	expression tag	UNP Q12888
A	1549	CYS	GLU	engineered mutation	UNP Q12888
A	1567	CYS	GLU	engineered mutation	UNP Q12888
B	1479	GLY	-	expression tag	UNP Q12888
B	1480	PRO	-	expression tag	UNP Q12888

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1481	GLY	-	expression tag	UNP Q12888
B	1482	HIS	-	expression tag	UNP Q12888
B	1483	MET	-	expression tag	UNP Q12888
B	1549	CYS	GLU	engineered mutation	UNP Q12888
B	1567	CYS	GLU	engineered mutation	UNP Q12888
C	1479	GLY	-	expression tag	UNP Q12888
C	1480	PRO	-	expression tag	UNP Q12888
C	1481	GLY	-	expression tag	UNP Q12888
C	1482	HIS	-	expression tag	UNP Q12888
C	1483	MET	-	expression tag	UNP Q12888
C	1549	CYS	GLU	engineered mutation	UNP Q12888
C	1567	CYS	GLU	engineered mutation	UNP Q12888
D	1479	GLY	-	expression tag	UNP Q12888
D	1480	PRO	-	expression tag	UNP Q12888
D	1481	GLY	-	expression tag	UNP Q12888
D	1482	HIS	-	expression tag	UNP Q12888
D	1483	MET	-	expression tag	UNP Q12888
D	1549	CYS	GLU	engineered mutation	UNP Q12888
D	1567	CYS	GLU	engineered mutation	UNP Q12888
E	1479	GLY	-	expression tag	UNP Q12888
E	1480	PRO	-	expression tag	UNP Q12888
E	1481	GLY	-	expression tag	UNP Q12888
E	1482	HIS	-	expression tag	UNP Q12888
E	1483	MET	-	expression tag	UNP Q12888
E	1549	CYS	GLU	engineered mutation	UNP Q12888
E	1567	CYS	GLU	engineered mutation	UNP Q12888
F	1479	GLY	-	expression tag	UNP Q12888
F	1480	PRO	-	expression tag	UNP Q12888
F	1481	GLY	-	expression tag	UNP Q12888
F	1482	HIS	-	expression tag	UNP Q12888
F	1483	MET	-	expression tag	UNP Q12888
F	1549	CYS	GLU	engineered mutation	UNP Q12888
F	1567	CYS	GLU	engineered mutation	UNP Q12888
G	1479	GLY	-	expression tag	UNP Q12888
G	1480	PRO	-	expression tag	UNP Q12888
G	1481	GLY	-	expression tag	UNP Q12888
G	1482	HIS	-	expression tag	UNP Q12888
G	1483	MET	-	expression tag	UNP Q12888
G	1549	CYS	GLU	engineered mutation	UNP Q12888
G	1567	CYS	GLU	engineered mutation	UNP Q12888
H	1479	GLY	-	expression tag	UNP Q12888
H	1480	PRO	-	expression tag	UNP Q12888

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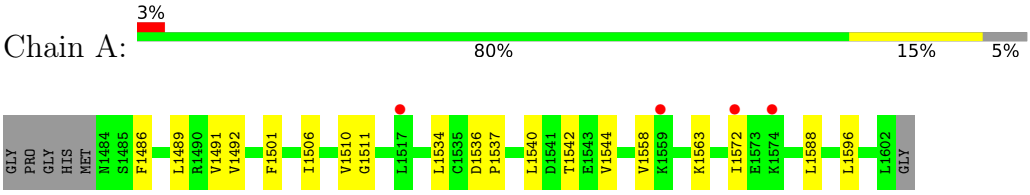
Chain	Residue	Modelled	Actual	Comment	Reference
H	1481	GLY	-	expression tag	UNP Q12888
H	1482	HIS	-	expression tag	UNP Q12888
H	1483	MET	-	expression tag	UNP Q12888
H	1549	CYS	GLU	engineered mutation	UNP Q12888
H	1567	CYS	GLU	engineered mutation	UNP Q12888
I	1479	GLY	-	expression tag	UNP Q12888
I	1480	PRO	-	expression tag	UNP Q12888
I	1481	GLY	-	expression tag	UNP Q12888
I	1482	HIS	-	expression tag	UNP Q12888
I	1483	MET	-	expression tag	UNP Q12888
I	1549	CYS	GLU	engineered mutation	UNP Q12888
I	1567	CYS	GLU	engineered mutation	UNP Q12888
J	1479	GLY	-	expression tag	UNP Q12888
J	1480	PRO	-	expression tag	UNP Q12888
J	1481	GLY	-	expression tag	UNP Q12888
J	1482	HIS	-	expression tag	UNP Q12888
J	1483	MET	-	expression tag	UNP Q12888
J	1549	CYS	GLU	engineered mutation	UNP Q12888
J	1567	CYS	GLU	engineered mutation	UNP Q12888

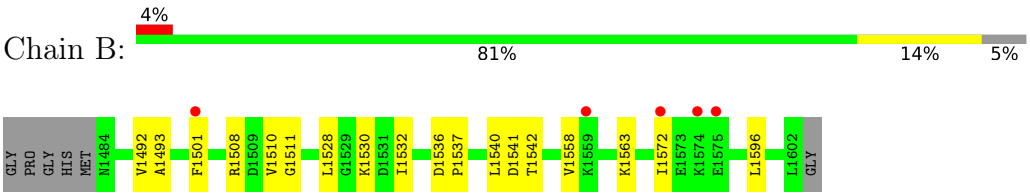
3 Residue-property plots (i)

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

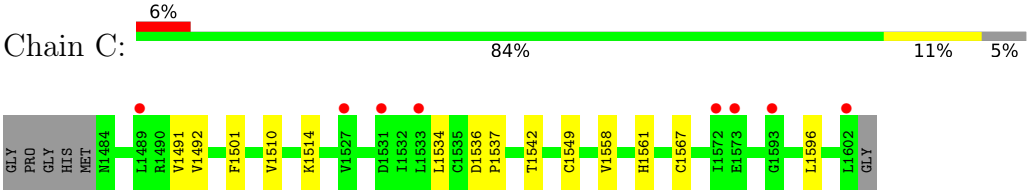
• Molecule 1: TP53-binding protein 1



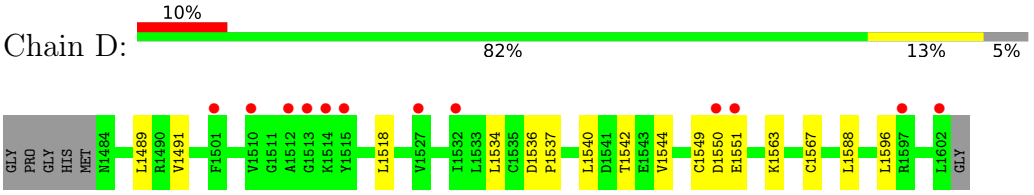
• Molecule 1: TP53-binding protein 1



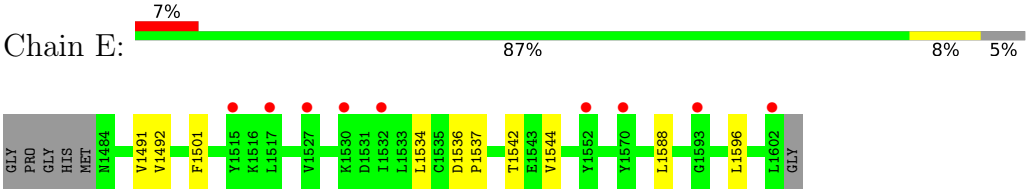
• Molecule 1: TP53-binding protein 1



• Molecule 1: TP53-binding protein 1

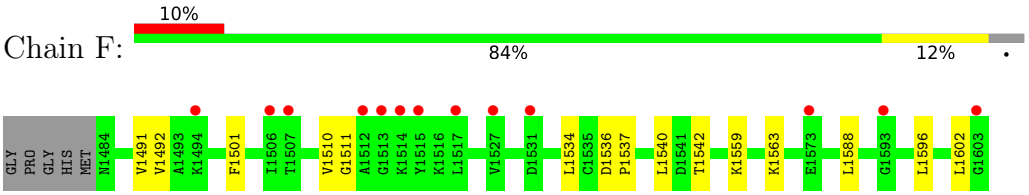


• Molecule 1: TP53-binding protein 1



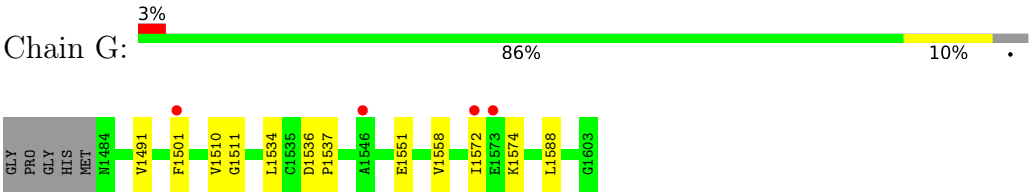
• Molecule 1: TP53-binding protein 1

Chain F:



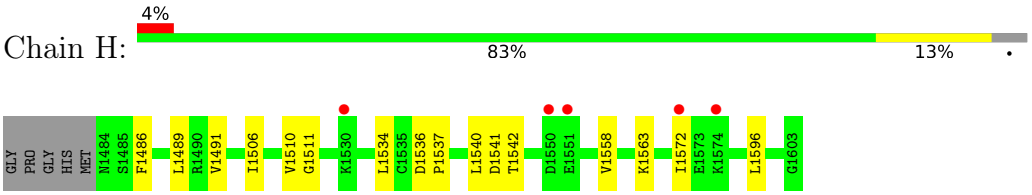
• Molecule 1: TP53-binding protein 1

Chain G:



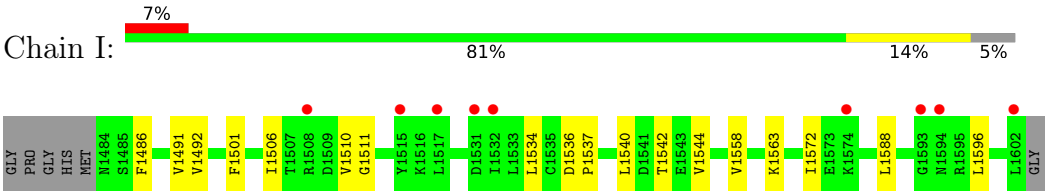
• Molecule 1: TP53-binding protein 1

Chain H:



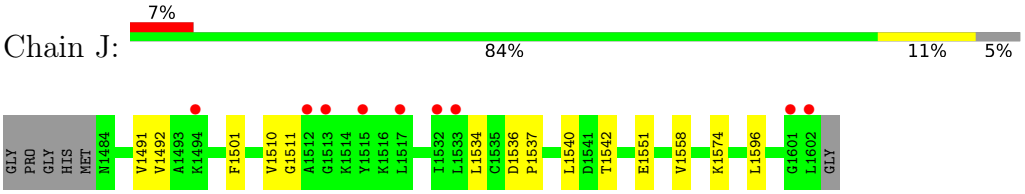
• Molecule 1: TP53-binding protein 1

Chain I:



• Molecule 1: TP53-binding protein 1

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.50Å 161.82Å 179.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 3.79 48.19 – 3.79	Depositor EDS
% Data completeness (in resolution range)	89.2 (48.19-3.79) 89.2 (48.19-3.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.300 0.255 , 0.305	Depositor DCC
R_{free} test set	1943 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	109.9	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 109.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	18847	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.25	0/968	0.49	0/1301
1	B	0.25	0/964	0.50	0/1295
1	C	0.24	0/964	0.50	0/1295
1	D	0.25	0/964	0.49	0/1295
1	E	0.25	0/968	0.50	0/1301
1	F	0.24	0/972	0.49	0/1306
1	G	0.24	0/972	0.49	0/1306
1	H	0.25	0/972	0.49	0/1306
1	I	0.25	0/968	0.50	0/1301
1	J	0.24	0/968	0.49	0/1301
All	All	0.25	0/9680	0.49	0/13007

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

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	949	936	936	16	0
1	B	945	932	931	12	0
1	C	945	932	931	9	0
1	D	945	932	931	15	0
1	E	949	936	936	6	0
1	F	953	939	939	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	953	939	939	7	0
1	H	953	939	939	13	0
1	I	949	936	936	13	0
1	J	949	936	936	9	0
All	All	9490	9357	9354	97	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 5.

All (97) 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:1540:LEU:HD21	1:F:1563:LYS:HB2	1.77	0.65
1:B:1508:ARG:NH1	1:D:1518:LEU:HD22	2.12	0.64
1:B:1563:LYS:HB2	1:I:1540:LEU:HD21	1.83	0.61
1:F:1542:THR:HG21	1:F:1596:LEU:HD11	1.83	0.60
1:D:1540:LEU:HD21	1:H:1563:LYS:HB2	1.83	0.60
1:I:1491:VAL:HG12	1:I:1534:LEU:HA	1.86	0.58
1:F:1588:LEU:HD11	1:F:1596:LEU:HD12	1.85	0.57
1:B:1540:LEU:HD21	1:I:1563:LYS:HB2	1.88	0.55
1:C:1491:VAL:HG12	1:C:1534:LEU:HD12	1.89	0.54
1:E:1544:VAL:HG12	1:E:1588:LEU:HD21	1.88	0.54
1:D:1491:VAL:HG12	1:D:1534:LEU:HA	1.89	0.54
1:B:1492:VAL:HG12	1:B:1501:PHE:HB3	1.89	0.53
1:E:1491:VAL:HG12	1:E:1534:LEU:HD12	1.91	0.53
1:A:1491:VAL:HG12	1:A:1534:LEU:HD12	1.92	0.51
1:I:1544:VAL:HG12	1:I:1588:LEU:HD21	1.93	0.51
1:E:1542:THR:HG21	1:E:1596:LEU:HD11	1.93	0.51
1:D:1563:LYS:HD2	1:H:1541:ASP:OD2	2.11	0.51
1:J:1491:VAL:HG12	1:J:1534:LEU:HA	1.93	0.51
1:F:1491:VAL:HG12	1:F:1534:LEU:HA	1.92	0.50
1:I:1492:VAL:HG12	1:I:1501:PHE:HB3	1.94	0.50
1:B:1542:THR:HG21	1:B:1596:LEU:HD11	1.93	0.49
1:A:1558:VAL:HG22	1:A:1572:ILE:CD1	2.42	0.49
1:C:1567:CYS:N	1:D:1549:CYS:SG	2.86	0.49
1:E:1491:VAL:HG12	1:E:1534:LEU:HA	1.96	0.48
1:G:1491:VAL:HG12	1:G:1534:LEU:HD12	1.95	0.47
1:E:1536:ASP:HB3	1:E:1537:PRO:HD3	1.97	0.47
1:A:1491:VAL:HG12	1:A:1534:LEU:HA	1.97	0.47
1:A:1588:LEU:CD1	1:A:1596:LEU:HD12	2.44	0.47
1:I:1491:VAL:HG12	1:I:1534:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1588:LEU:HD11	1:A:1596:LEU:HD12	1.97	0.47
1:H:1542:THR:HG21	1:H:1596:LEU:HD11	1.96	0.47
1:J:1491:VAL:HG12	1:J:1534:LEU:HD12	1.95	0.47
1:C:1536:ASP:HB3	1:C:1537:PRO:HD3	1.97	0.46
1:A:1492:VAL:HG12	1:A:1501:PHE:HB3	1.96	0.46
1:G:1491:VAL:HG12	1:G:1534:LEU:HA	1.97	0.46
1:B:1508:ARG:HH11	1:D:1518:LEU:HD22	1.81	0.46
1:I:1536:ASP:HB3	1:I:1537:PRO:HD3	1.98	0.46
1:A:1563:LYS:HB2	1:F:1540:LEU:HD21	1.97	0.46
1:H:1558:VAL:HG22	1:H:1572:ILE:CD1	2.46	0.45
1:F:1492:VAL:HG12	1:F:1501:PHE:HB3	1.97	0.45
1:H:1486:PHE:O	1:H:1506:ILE:HG21	2.15	0.45
1:B:1528:LEU:HD12	1:B:1530:LYS:HE2	1.98	0.45
1:A:1544:VAL:HG12	1:A:1588:LEU:HD21	1.98	0.45
1:A:1486:PHE:O	1:A:1506:ILE:HG21	2.16	0.45
1:C:1492:VAL:HG12	1:C:1501:PHE:HB3	1.99	0.45
1:I:1558:VAL:HG22	1:I:1572:ILE:CD1	2.46	0.45
1:C:1491:VAL:HG12	1:C:1534:LEU:HA	1.98	0.44
1:C:1542:THR:HG21	1:C:1596:LEU:HD11	1.99	0.44
1:J:1492:VAL:HG12	1:J:1501:PHE:HB3	1.98	0.44
1:J:1536:ASP:HB3	1:J:1537:PRO:HD3	1.99	0.44
1:G:1536:ASP:HB3	1:G:1537:PRO:HD3	1.99	0.44
1:F:1536:ASP:HB3	1:F:1537:PRO:HD3	2.00	0.44
1:C:1558:VAL:HG11	1:C:1561:HIS:HE1	1.83	0.44
1:D:1536:ASP:HB3	1:D:1537:PRO:HD3	2.00	0.44
1:A:1542:THR:HG21	1:A:1596:LEU:HD11	2.00	0.44
1:F:1491:VAL:HG12	1:F:1534:LEU:HD12	2.00	0.44
1:H:1489:LEU:N	1:H:1489:LEU:HD12	2.33	0.44
1:H:1536:ASP:HB3	1:H:1537:PRO:HD3	1.98	0.44
1:C:1510:VAL:HB	1:C:1514:LYS:O	2.18	0.43
1:D:1544:VAL:HG12	1:D:1588:LEU:HD21	2.00	0.43
1:B:1510:VAL:HG12	1:B:1511:GLY:H	1.84	0.43
1:I:1542:THR:HG21	1:I:1596:LEU:HD11	1.99	0.43
1:B:1536:ASP:HB3	1:B:1537:PRO:HD3	1.99	0.43
1:H:1510:VAL:HG12	1:H:1511:GLY:H	1.83	0.43
1:A:1486:PHE:HA	1:A:1489:LEU:HD13	2.00	0.43
1:B:1558:VAL:HG22	1:B:1572:ILE:CD1	2.49	0.43
1:D:1491:VAL:HG12	1:D:1534:LEU:HD12	2.01	0.43
1:D:1550:ASP:O	1:D:1551:GLU:HB2	2.19	0.43
1:H:1491:VAL:HG12	1:H:1534:LEU:HA	2.01	0.42
1:C:1549:CYS:SG	1:D:1567:CYS:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1486:PHE:O	1:I:1506:ILE:HG21	2.19	0.42
1:F:1510:VAL:HG12	1:F:1511:GLY:H	1.84	0.42
1:H:1486:PHE:HA	1:H:1489:LEU:HD13	2.01	0.42
1:B:1541:ASP:OD2	1:I:1563:LYS:HD2	2.19	0.42
1:J:1510:VAL:HG12	1:J:1511:GLY:H	1.85	0.42
1:D:1563:LYS:HB3	1:H:1540:LEU:HD21	2.00	0.42
1:D:1542:THR:HG21	1:D:1596:LEU:HD11	2.02	0.42
1:D:1489:LEU:N	1:D:1489:LEU:HD12	2.35	0.41
1:J:1551:GLU:HG2	1:J:1574:LYS:HD2	2.02	0.41
1:A:1536:ASP:HB3	1:A:1537:PRO:HD3	2.02	0.41
1:D:1563:LYS:CB	1:H:1540:LEU:HD21	2.49	0.41
1:G:1510:VAL:HG12	1:G:1511:GLY:H	1.85	0.41
1:J:1540:LEU:HD12	1:J:1558:VAL:HG12	2.02	0.41
1:E:1492:VAL:HG12	1:E:1501:PHE:HB3	2.03	0.41
1:G:1551:GLU:HG2	1:G:1574:LYS:HD2	2.02	0.41
1:A:1510:VAL:HG12	1:A:1511:GLY:H	1.86	0.41
1:B:1493:ALA:HB2	1:B:1532:ILE:HA	2.02	0.41
1:I:1510:VAL:HG12	1:I:1511:GLY:H	1.85	0.41
1:J:1542:THR:HG21	1:J:1596:LEU:HD11	2.02	0.41
1:I:1491:VAL:HG11	1:I:1506:ILE:HD11	2.03	0.41
1:A:1489:LEU:HD12	1:A:1489:LEU:N	2.36	0.40
1:A:1563:LYS:O	1:F:1559:LYS:HE3	2.21	0.40
1:G:1501:PHE:HB2	1:G:1588:LEU:HB2	2.03	0.40
1:H:1491:VAL:HG12	1:H:1534:LEU:HD12	2.04	0.40
1:F:1534:LEU:HB2	1:F:1602:LEU:HD21	2.03	0.40
1:G:1558:VAL:HG22	1:G:1572:ILE:CD1	2.52	0.40
1:J:1491:VAL:CG1	1:J:1534:LEU:HD12	2.51	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	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
1	B	117/125 (94%)	114 (97%)	3 (3%)	0	100	100
1	C	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
1	D	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
1	E	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
1	F	118/125 (94%)	115 (98%)	3 (2%)	0	100	100
1	G	118/125 (94%)	115 (98%)	3 (2%)	0	100	100
1	H	118/125 (94%)	116 (98%)	2 (2%)	0	100	100
1	I	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
1	J	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
All	All	1173/1250 (94%)	1153 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	101/104 (97%)	101 (100%)	0	100	100
1	B	100/104 (96%)	100 (100%)	0	100	100
1	C	100/104 (96%)	100 (100%)	0	100	100
1	D	100/104 (96%)	100 (100%)	0	100	100
1	E	101/104 (97%)	101 (100%)	0	100	100
1	F	101/104 (97%)	101 (100%)	0	100	100
1	G	101/104 (97%)	101 (100%)	0	100	100
1	H	101/104 (97%)	101 (100%)	0	100	100
1	I	101/104 (97%)	101 (100%)	0	100	100
1	J	101/104 (97%)	101 (100%)	0	100	100
All	All	1007/1040 (97%)	1007 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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^{th} 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	119/125 (95%)	0.44	4 (3%) 45 37	102, 131, 167, 207	0
1	B	119/125 (95%)	0.44	5 (4%) 36 30	108, 134, 174, 200	0
1	C	119/125 (95%)	0.56	8 (6%) 17 14	116, 138, 168, 177	0
1	D	119/125 (95%)	0.67	12 (10%) 7 6	111, 134, 181, 213	0
1	E	119/125 (95%)	0.60	9 (7%) 13 11	110, 143, 181, 219	0
1	F	120/125 (96%)	0.71	13 (10%) 5 5	105, 141, 188, 209	0
1	G	120/125 (96%)	0.46	4 (3%) 46 38	111, 133, 170, 195	0
1	H	120/125 (96%)	0.56	5 (4%) 36 30	114, 136, 170, 227	0
1	I	119/125 (95%)	0.64	9 (7%) 13 11	119, 150, 188, 195	0
1	J	119/125 (95%)	0.64	9 (7%) 13 11	125, 152, 193, 215	0
All	All	1193/1250 (95%)	0.57	78 (6%) 18 14	102, 139, 181, 227	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1602	LEU	4.7
1	D	1501	PHE	4.3
1	F	1513	GLY	4.3
1	I	1532	ILE	4.1
1	D	1550	ASP	3.7
1	I	1602	LEU	3.6
1	E	1593	GLY	3.4
1	F	1593	GLY	3.1
1	I	1593	GLY	3.1
1	F	1517	LEU	3.1
1	F	1512	ALA	3.1
1	F	1531	ASP	3.0
1	B	1574	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	1515	TYR	3.0
1	F	1515	TYR	2.8
1	C	1593	GLY	2.8
1	D	1513	GLY	2.8
1	F	1506	ILE	2.7
1	I	1594	ASN	2.7
1	E	1602	LEU	2.6
1	E	1517	LEU	2.6
1	H	1551	GLU	2.6
1	F	1514	LYS	2.6
1	D	1514	LYS	2.6
1	E	1515	TYR	2.6
1	J	1517	LEU	2.6
1	D	1512	ALA	2.5
1	H	1550	ASP	2.5
1	J	1515	TYR	2.5
1	I	1508	ARG	2.5
1	A	1559	LYS	2.5
1	D	1551	GLU	2.5
1	C	1527	VAL	2.4
1	H	1572	ILE	2.4
1	B	1572	ILE	2.4
1	F	1507	THR	2.4
1	J	1532	ILE	2.4
1	E	1570	TYR	2.4
1	E	1532	ILE	2.4
1	I	1517	LEU	2.4
1	B	1575	GLU	2.4
1	C	1533	LEU	2.4
1	H	1574	LYS	2.4
1	C	1602	LEU	2.4
1	J	1533	LEU	2.3
1	J	1512	ALA	2.3
1	D	1602	LEU	2.3
1	F	1527	VAL	2.3
1	D	1597	ARG	2.3
1	H	1530	LYS	2.3
1	A	1572	ILE	2.3
1	F	1603	GLY	2.3
1	J	1601	GLY	2.3
1	I	1574	LYS	2.3
1	C	1573	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	1494	LYS	2.2
1	G	1573	GLU	2.2
1	D	1527	VAL	2.2
1	G	1501	PHE	2.2
1	J	1513	GLY	2.2
1	I	1531	ASP	2.2
1	D	1532	ILE	2.2
1	D	1510	VAL	2.1
1	C	1572	ILE	2.1
1	G	1572	ILE	2.1
1	F	1573	GLU	2.1
1	E	1552	TYR	2.1
1	C	1489	LEU	2.1
1	D	1515	TYR	2.1
1	B	1501	PHE	2.1
1	A	1574	LYS	2.1
1	J	1494	LYS	2.1
1	A	1517	LEU	2.0
1	G	1546	ALA	2.0
1	E	1527	VAL	2.0
1	B	1559	LYS	2.0
1	E	1530	LYS	2.0
1	C	1531	ASP	2.0

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 monosaccharides 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.