



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2016 – 02:33 PM EDT

PDB ID : 5IGQ
Title : WD40 domain of Human E3 Ubiquitin Ligase COP1 (RFWD2) bound to peptide from Trib1
Authors : Uljon, S.; Blacklow, S.C.
Deposited on : 2016-02-28
Resolution : 3.90 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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-20027457

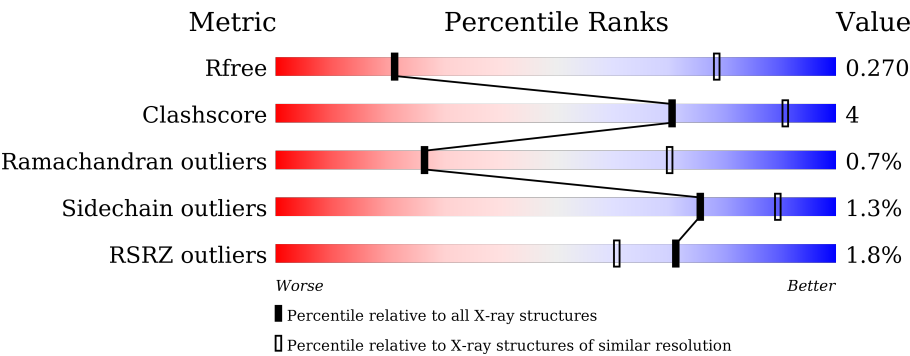
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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.

Mol	Chain	Length	Quality of chain
1	A	353	<div><div></div><div>78%14%8%</div></div>
1	B	353	<div><div>%</div><div>79%12%8%</div></div>
1	C	353	<div><div>2%</div><div>81%10%8%</div></div>
1	D	353	<div><div>%</div><div>82%9%8%</div></div>
1	E	353	<div><div>%</div><div>78%13%8%</div></div>
1	F	353	<div><div>3%</div><div>78%14%8%</div></div>

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Mol	Chain	Length	Quality of chain
2	U	11	<div><div></div><div>73%</div><div>27%</div></div>
3	V	8	<div><div>25%</div><div>75%</div><div>25%</div></div>
3	W	8	<div><div>25%</div><div>100%</div><div></div></div>
3	X	8	<div><div></div><div>75%</div><div>25%</div></div>
3	Y	8	<div><div>13%</div><div>100%</div><div></div></div>
3	Z	8	<div><div>13%</div><div>100%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15349 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 E3 ubiquitin-protein ligase RFWD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	1	0
			2487	1586	413	472	16			
1	B	324	Total	C	N	O	S	0	1	0
			2487	1586	413	472	16			
1	C	324	Total	C	N	O	S	0	1	0
			2487	1586	413	472	16			
1	D	324	Total	C	N	O	S	0	1	0
			2487	1586	413	472	16			
1	E	324	Total	C	N	O	S	0	1	0
			2487	1586	413	472	16			
1	F	324	Total	C	N	O	S	0	1	0
			2487	1586	413	472	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	MET	-	expression tag	UNP Q8NHY2
A	380	HIS	-	expression tag	UNP Q8NHY2
A	381	HIS	-	expression tag	UNP Q8NHY2
A	382	HIS	-	expression tag	UNP Q8NHY2
A	383	HIS	-	expression tag	UNP Q8NHY2
A	384	HIS	-	expression tag	UNP Q8NHY2
A	385	HIS	-	expression tag	UNP Q8NHY2
B	379	MET	-	expression tag	UNP Q8NHY2
B	380	HIS	-	expression tag	UNP Q8NHY2
B	381	HIS	-	expression tag	UNP Q8NHY2
B	382	HIS	-	expression tag	UNP Q8NHY2
B	383	HIS	-	expression tag	UNP Q8NHY2
B	384	HIS	-	expression tag	UNP Q8NHY2
B	385	HIS	-	expression tag	UNP Q8NHY2
C	379	MET	-	expression tag	UNP Q8NHY2
C	380	HIS	-	expression tag	UNP Q8NHY2
C	381	HIS	-	expression tag	UNP Q8NHY2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	382	HIS	-	expression tag	UNP Q8NHY2
C	383	HIS	-	expression tag	UNP Q8NHY2
C	384	HIS	-	expression tag	UNP Q8NHY2
C	385	HIS	-	expression tag	UNP Q8NHY2
D	379	MET	-	expression tag	UNP Q8NHY2
D	380	HIS	-	expression tag	UNP Q8NHY2
D	381	HIS	-	expression tag	UNP Q8NHY2
D	382	HIS	-	expression tag	UNP Q8NHY2
D	383	HIS	-	expression tag	UNP Q8NHY2
D	384	HIS	-	expression tag	UNP Q8NHY2
D	385	HIS	-	expression tag	UNP Q8NHY2
E	379	MET	-	expression tag	UNP Q8NHY2
E	380	HIS	-	expression tag	UNP Q8NHY2
E	381	HIS	-	expression tag	UNP Q8NHY2
E	382	HIS	-	expression tag	UNP Q8NHY2
E	383	HIS	-	expression tag	UNP Q8NHY2
E	384	HIS	-	expression tag	UNP Q8NHY2
E	385	HIS	-	expression tag	UNP Q8NHY2
F	379	MET	-	expression tag	UNP Q8NHY2
F	380	HIS	-	expression tag	UNP Q8NHY2
F	381	HIS	-	expression tag	UNP Q8NHY2
F	382	HIS	-	expression tag	UNP Q8NHY2
F	383	HIS	-	expression tag	UNP Q8NHY2
F	384	HIS	-	expression tag	UNP Q8NHY2
F	385	HIS	-	expression tag	UNP Q8NHY2

- Molecule 2 is a protein called Tribbles homolog 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	11	Total	C	N	O	0	0	0
			92	56	13	23			

- Molecule 3 is a protein called Tribbles homolog 1.

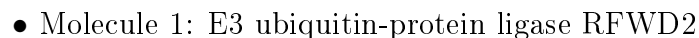
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	V	8	Total	C	N	O	0	0	0
			67	42	9	16			
3	W	8	Total	C	N	O	0	0	0
			67	42	9	16			
3	X	8	Total	C	N	O	0	0	0
			67	42	9	16			

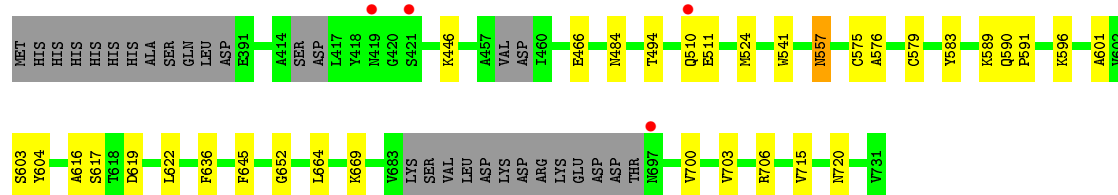
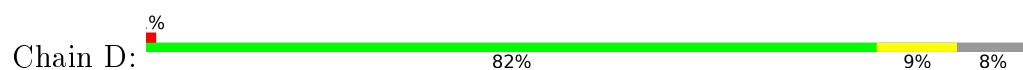
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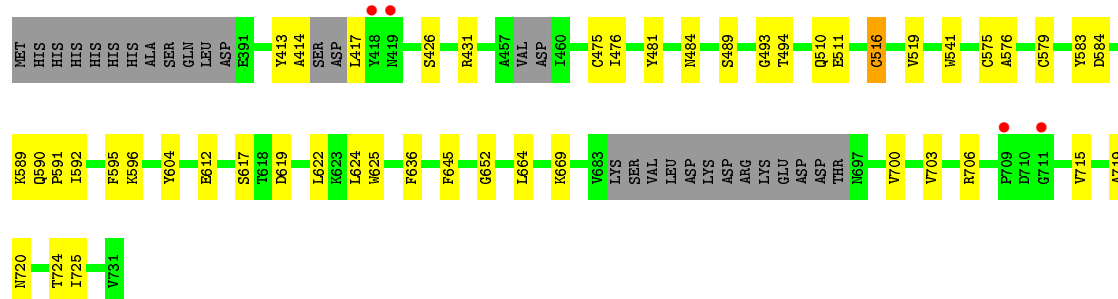
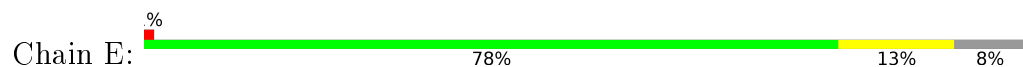
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Y	8	Total	C	N	O	0	0	0
			67	42	9	16			
3	Z	8	Total	C	N	O	0	0	0
			67	42	9	16			

- Molecule 1: E3 ubiquitin-protein ligase RFWD2

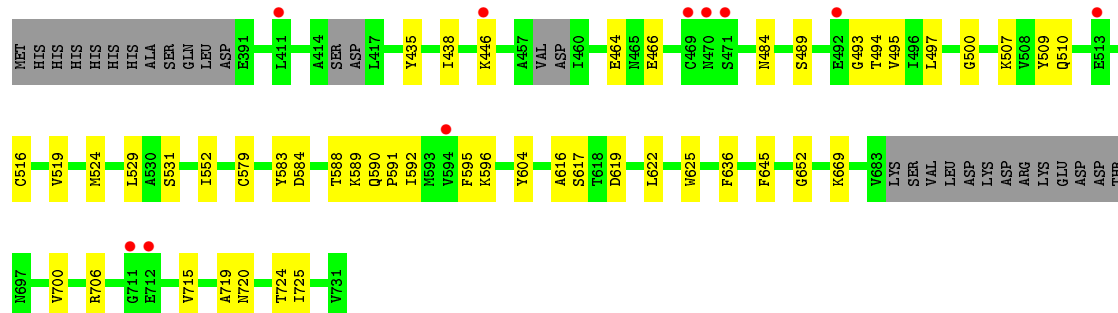
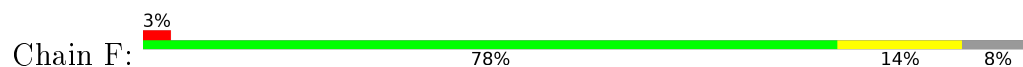




- Molecule 1: E3 ubiquitin-protein ligase RFWD2



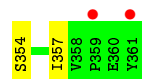
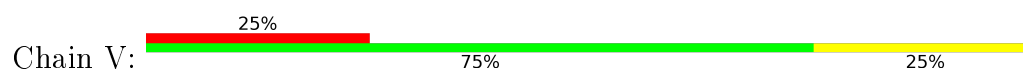
- Molecule 1: E3 ubiquitin-protein ligase RFWD2



- Molecule 2: Tribbles homolog 1



- Molecule 3: Tribbles homolog 1




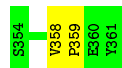
- Molecule 3: Tribbles homolog 1

Chain W:  25% 100%



- Molecule 3: Tribbles homolog 1

Chain X:  75% 25%



- Molecule 3: Tribbles homolog 1

Chain Y:  13% 100%



- Molecule 3: Tribbles homolog 1

Chain Z:  13% 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	247.65Å 249.58Å 124.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 3.90 29.40 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.77-3.90) 86.5 (29.40-3.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.86Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.228 , 0.277 0.224 , 0.270	Depositor DCC
R_{free} test set	1548 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	130.2	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15349	wwPDB-VP
Average B, all atoms (Å ²)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.375 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	0.25	0/2546	0.49	1/3452 (0.0%)
1	B	0.25	0/2546	0.48	1/3452 (0.0%)
1	C	0.25	0/2546	0.49	1/3452 (0.0%)
1	D	0.25	0/2546	0.49	1/3452 (0.0%)
1	E	0.25	0/2546	0.49	1/3452 (0.0%)
1	F	0.25	0/2546	0.48	1/3452 (0.0%)
2	U	0.35	0/93	0.65	0/126
3	V	0.25	0/68	0.39	0/91
3	W	0.25	0/68	0.39	0/91
3	X	0.26	0/68	0.50	0/91
3	Y	0.25	0/68	0.38	0/91
3	Z	0.25	0/68	0.40	0/91
All	All	0.25	0/15709	0.49	6/21293 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	589	LYS	C-N-CA	5.95	136.57	121.70
1	A	589	LYS	C-N-CA	5.87	136.38	121.70
1	F	589	LYS	C-N-CA	5.76	136.09	121.70
1	C	589	LYS	C-N-CA	5.70	135.95	121.70
1	B	589	LYS	C-N-CA	5.67	135.87	121.70
1	D	589	LYS	C-N-CA	5.64	135.81	121.70

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	2487	0	2348	24	0
1	B	2487	0	2348	21	0
1	C	2487	0	2348	20	0
1	D	2487	0	2348	19	0
1	E	2487	0	2348	23	0
1	F	2487	0	2348	23	0
2	U	92	0	76	2	0
3	V	67	0	58	1	0
3	W	67	0	58	0	0
3	X	67	0	58	3	0
3	Y	67	0	58	0	0
3	Z	67	0	58	0	0
All	All	15349	0	14454	132	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 4.

All (132) 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:E:622:LEU:HB2	1:E:636:PHE:HB2	1.63	0.78
2:U:362:GLN:HB2	2:U:363:GLU:HA	1.72	0.71
1:D:622:LEU:HB2	1:D:636:PHE:HB2	1.71	0.71
1:F:622:LEU:HB2	1:F:636:PHE:HB2	1.72	0.71
1:A:700:VAL:HA	1:A:720:ASN:HA	1.74	0.70
1:C:622:LEU:HB2	1:C:636:PHE:HB2	1.72	0.70
1:B:622:LEU:HB2	1:B:636:PHE:HB2	1.75	0.69
1:D:601:ALA:HB3	3:X:358:VAL:HG13	1.75	0.68
1:A:622:LEU:HB2	1:A:636:PHE:HB2	1.79	0.64
1:D:700:VAL:HA	1:D:720:ASN:HA	1.83	0.59
1:F:617:SER:OG	1:F:619:ASP:OD1	2.20	0.59
1:F:700:VAL:HA	1:F:720:ASN:HA	1.85	0.59
1:C:617:SER:OG	1:C:619:ASP:OD1	2.22	0.58
1:A:617:SER:OG	1:A:619:ASP:OD1	2.22	0.57
1:C:612:GLU:HB3	1:C:624:LEU:HD11	1.86	0.57
1:A:664:LEU:HD13	1:A:703:VAL:HG11	1.86	0.56
1:A:465:ASN:ND2	1:A:501:PHE:O	2.39	0.56
1:D:576:ALA:HA	1:D:601:ALA:HB1	1.87	0.55
1:E:700:VAL:HA	1:E:720:ASN:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ILE:HD13	1:A:725:ILE:HD13	1.87	0.55
1:D:617:SER:OG	1:D:619:ASP:OD1	2.24	0.54
1:C:494:THR:HG23	1:C:510:GLN:HG2	1.88	0.54
1:E:511:GLU:HB2	1:E:541:TRP:HH2	1.73	0.53
1:E:617:SER:OG	1:E:619:ASP:OD1	2.26	0.53
1:C:706:ARG:HB3	1:C:715:VAL:HG13	1.90	0.53
1:C:427:ILE:HG12	1:C:438:ILE:HG12	1.90	0.52
1:A:604:TYR:HB2	1:A:616:ALA:HB3	1.91	0.52
1:D:583:TYR:CZ	1:D:591:PRO:HB3	2.45	0.52
1:E:494:THR:HG23	1:E:510:GLN:HG2	1.90	0.52
1:A:552:ILE:HG12	1:A:588:THR:HB	1.92	0.52
1:C:489:SER:HB3	1:C:519:VAL:HG13	1.92	0.51
1:A:489:SER:HB3	1:A:519:VAL:HG13	1.92	0.51
1:B:700:VAL:HA	1:B:720:ASN:HA	1.93	0.51
1:F:446:LYS:HG2	1:F:466:GLU:HG3	1.93	0.51
1:A:493:GLY:HA2	1:A:516:CYS:HB2	1.91	0.51
1:E:624:LEU:HB2	1:E:636:PHE:HE1	1.76	0.50
1:D:579:CYS:SG	1:D:596:LYS:HG2	2.51	0.50
1:B:706:ARG:HB3	1:B:715:VAL:HG13	1.93	0.50
1:A:519:VAL:HG12	1:A:531:SER:HB3	1.93	0.50
1:B:617:SER:OG	1:B:619:ASP:OD1	2.29	0.50
1:F:583:TYR:CZ	1:F:591:PRO:HB3	2.47	0.50
1:D:494:THR:HG23	1:D:510:GLN:HG2	1.93	0.49
1:D:601:ALA:HB3	3:X:358:VAL:CG1	2.41	0.49
1:F:584:ASP:HB2	1:F:592:ILE:HD11	1.93	0.49
1:D:446:LYS:HG2	1:D:466:GLU:HG3	1.95	0.49
1:E:431:ARG:NH1	1:E:481:TYR:O	2.44	0.49
1:C:579:CYS:SG	1:C:596:LYS:HG2	2.53	0.49
1:D:706:ARG:HB3	1:D:715:VAL:HG13	1.94	0.49
1:A:595:PHE:HB3	1:A:625:TRP:CE3	2.48	0.48
1:E:579:CYS:SG	1:E:596:LYS:HG2	2.53	0.48
1:C:557:ASN:O	1:C:576:ALA:N	2.41	0.48
1:C:580:VAL:HG22	1:C:602:VAL:HG11	1.95	0.48
1:B:595:PHE:HB3	1:B:625:TRP:CE3	2.48	0.48
1:D:604:TYR:HB2	1:D:616:ALA:HB3	1.96	0.48
1:F:497:LEU:HD12	1:F:507:LYS:HB2	1.96	0.48
1:A:706:ARG:HB3	1:A:715:VAL:HG13	1.95	0.48
1:C:604:TYR:OH	1:C:645:PHE:HB3	2.14	0.47
1:E:706:ARG:HB3	1:E:715:VAL:HG13	1.95	0.47
2:U:362:GLN:CB	2:U:363:GLU:HA	2.41	0.47
1:B:580:VAL:HB	1:B:595:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ARG:HH12	1:C:408:LEU:HB2	1.80	0.47
1:A:446:LYS:HG2	1:A:466:GLU:HG3	1.96	0.47
1:B:579:CYS:SG	1:B:596:LYS:HG2	2.55	0.47
1:F:493:GLY:HA2	1:F:516:CYS:HB2	1.96	0.47
1:B:426:SER:HB3	1:B:476:ILE:HG12	1.97	0.47
1:F:604:TYR:HB2	1:F:616:ALA:HB3	1.96	0.47
1:E:583:TYR:CZ	1:E:591:PRO:HB3	2.50	0.46
1:B:583:TYR:CZ	1:B:591:PRO:HB3	2.50	0.46
1:B:664:LEU:HD13	1:B:703:VAL:HG11	1.97	0.46
1:C:583:TYR:CZ	1:C:591:PRO:HB3	2.50	0.46
1:F:706:ARG:HB3	1:F:715:VAL:HG13	1.98	0.46
1:A:583:TYR:CE1	1:A:591:PRO:HB3	2.50	0.46
1:E:493:GLY:HA2	1:E:516:CYS:HB2	1.98	0.46
1:F:519:VAL:HG12	1:F:531:SER:HB3	1.97	0.46
1:B:552:ILE:HG12	1:B:588:THR:HB	1.98	0.46
1:B:604:TYR:HB2	1:B:616:ALA:HB3	1.98	0.46
1:E:719:ALA:HA	1:E:724:THR:O	2.15	0.46
1:B:414:ALA:HB1	1:B:417:LEU:N	2.32	0.45
1:D:511:GLU:HB2	1:D:541:TRP:HH2	1.80	0.45
1:E:612:GLU:HB3	1:E:624:LEU:HD11	1.98	0.45
1:C:604:TYR:HB2	1:C:616:ALA:HB3	1.99	0.45
1:E:575:CYS:SG	1:E:576:ALA:N	2.90	0.45
1:D:604:TYR:OH	1:D:645:PHE:HB3	2.17	0.45
1:B:583:TYR:CE1	1:B:591:PRO:HB3	2.52	0.44
1:C:583:TYR:CE1	1:C:591:PRO:HB3	2.52	0.44
1:F:604:TYR:OH	1:F:645:PHE:HB3	2.17	0.44
1:E:426:SER:HB3	1:E:476:ILE:HG12	1.97	0.44
1:F:552:ILE:HG12	1:F:588:THR:HB	1.98	0.44
1:F:494:THR:HG23	1:F:510:GLN:HG2	1.98	0.44
1:F:595:PHE:HB3	1:F:625:TRP:CE3	2.53	0.44
1:A:604:TYR:OH	1:A:645:PHE:HB3	2.18	0.44
1:E:584:ASP:HB2	1:E:592:ILE:HD11	2.00	0.44
1:F:489:SER:HB3	1:F:519:VAL:HG13	2.00	0.44
1:A:584:ASP:HB2	1:A:592:ILE:HD11	1.99	0.44
1:C:700:VAL:HA	1:C:720:ASN:HA	1.99	0.44
1:D:557:ASN:O	1:D:576:ALA:N	2.46	0.43
1:A:579:CYS:SG	1:A:596:LYS:HG2	2.58	0.43
1:E:664:LEU:HD13	1:E:703:VAL:HG11	2.00	0.43
1:B:426:SER:HB2	1:B:475:CYS:HA	1.99	0.43
1:B:519:VAL:HG12	1:B:531:SER:HB3	1.99	0.43
1:A:583:TYR:CZ	1:A:591:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:SER:HB3	1:C:485:LEU:HB3	2.00	0.43
1:A:580:VAL:HG22	1:A:602:VAL:HG11	2.01	0.43
1:F:435:TYR:HE2	1:F:464:GLU:HG2	1.84	0.43
1:D:664:LEU:HD13	1:D:703:VAL:HG11	1.99	0.43
1:E:414:ALA:HB1	1:E:417:LEU:N	2.34	0.43
1:A:495:VAL:HB	1:A:509:TYR:HB2	2.01	0.42
1:D:603:SER:HB3	3:X:358:VAL:CG2	2.49	0.42
1:C:529:LEU:O	1:C:540:LEU:HD13	2.20	0.42
1:A:497:LEU:HD12	1:A:507:LYS:HB2	2.00	0.42
1:F:495:VAL:HB	1:F:509:TYR:HB2	2.01	0.42
1:D:575:CYS:SG	1:D:576:ALA:N	2.92	0.42
1:E:489:SER:HB3	1:E:519:VAL:HG13	2.01	0.42
1:E:604:TYR:OH	1:E:645:PHE:HB3	2.20	0.42
3:V:354:SER:HB2	3:V:357:ILE:HD11	2.02	0.42
1:E:595:PHE:HB3	1:E:625:TRP:CE3	2.55	0.42
1:B:438:ILE:HD13	1:B:725:ILE:HD13	2.01	0.42
1:E:413:TYR:HB2	1:E:725:ILE:HD11	2.01	0.42
1:F:438:ILE:HD13	1:F:725:ILE:HD13	2.02	0.41
1:A:614:VAL:HG21	1:A:655:ILE:HD13	2.03	0.41
1:E:426:SER:HB2	1:E:475:CYS:HA	2.01	0.41
1:F:579:CYS:SG	1:F:596:LYS:HG2	2.60	0.41
1:B:511:GLU:HB2	1:B:541:TRP:HH2	1.85	0.41
1:C:519:VAL:HG12	1:C:531:SER:HB3	2.02	0.41
1:F:435:TYR:CE2	1:F:464:GLU:HG2	2.55	0.41
1:F:596:LYS:HE2	1:F:596:LYS:HB3	1.89	0.41
1:B:493:GLY:HA2	1:B:516:CYS:HB2	2.01	0.41
1:C:598:HIS:CG	1:C:617:SER:HG	2.35	0.41
1:F:719:ALA:HA	1:F:724:THR:O	2.20	0.41
1:B:717:ILE:HG12	1:B:727:VAL:HG22	2.03	0.40
1:D:596:LYS:HB3	1:D:596:LYS:HE2	1.90	0.40
1:B:497:LEU:HD12	1:B:507:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	317/353 (90%)	303 (96%)	12 (4%)	2 (1%)	30	73
1	B	317/353 (90%)	300 (95%)	15 (5%)	2 (1%)	30	73
1	C	317/353 (90%)	298 (94%)	18 (6%)	1 (0%)	46	82
1	D	317/353 (90%)	296 (93%)	19 (6%)	2 (1%)	30	73
1	E	317/353 (90%)	295 (93%)	20 (6%)	2 (1%)	30	73
1	F	317/353 (90%)	300 (95%)	14 (4%)	3 (1%)	21	65
2	U	9/11 (82%)	7 (78%)	2 (22%)	0	100	100
3	V	6/8 (75%)	6 (100%)	0	0	100	100
3	W	6/8 (75%)	6 (100%)	0	0	100	100
3	X	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	4
3	Y	6/8 (75%)	6 (100%)	0	0	100	100
3	Z	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1941/2169 (90%)	1827 (94%)	101 (5%)	13 (1%)	26	70

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	GLN
1	A	652	GLY
3	X	359	PRO
1	E	590	GLN
1	C	590	GLN
1	D	652	GLY
1	E	652	GLY
1	F	590	GLN
1	B	590	GLN
1	F	500	GLY
1	D	590	GLN
1	F	652	GLY
1	B	652	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	263/313 (84%)	260 (99%)	3 (1%)	80	90
1	B	263/313 (84%)	260 (99%)	3 (1%)	80	90
1	C	263/313 (84%)	260 (99%)	3 (1%)	80	90
1	D	263/313 (84%)	259 (98%)	4 (2%)	72	89
1	E	263/313 (84%)	260 (99%)	3 (1%)	80	90
1	F	263/313 (84%)	259 (98%)	4 (2%)	72	89
2	U	11/11 (100%)	10 (91%)	1 (9%)	12	47
3	V	8/8 (100%)	8 (100%)	0	100	100
3	W	8/8 (100%)	8 (100%)	0	100	100
3	X	8/8 (100%)	8 (100%)	0	100	100
3	Y	8/8 (100%)	8 (100%)	0	100	100
3	Z	8/8 (100%)	8 (100%)	0	100	100
All	All	1629/1929 (84%)	1608 (99%)	21 (1%)	76	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	524	MET
1	A	669	LYS
2	U	364	ASP
1	B	484	ASN
1	B	584	ASP
1	B	669	LYS
1	C	484	ASN
1	C	529	LEU
1	C	669	LYS
1	D	484	ASN
1	D	524	MET
1	D	557	ASN
1	D	669	LYS
1	E	484	ASN
1	E	516	CYS
1	E	669	LYS
1	F	484	ASN
1	F	524	MET

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Mol	Chain	Res	Type
1	F	529	LEU
1	F	669	LYS

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 [i](#)

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, 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	324/353 (91%)	-0.49	0 100 100	113, 166, 232, 295	0
1	B	324/353 (91%)	-0.49	5 (1%) 76 66	100, 171, 234, 313	0
1	C	324/353 (91%)	-0.36	7 (2%) 65 54	119, 192, 264, 315	0
1	D	324/353 (91%)	-0.38	4 (1%) 81 72	107, 182, 256, 313	0
1	E	324/353 (91%)	-0.34	4 (1%) 81 72	115, 187, 248, 336	0
1	F	324/353 (91%)	-0.32	10 (3%) 52 40	127, 194, 265, 329	0
2	U	11/11 (100%)	-0.34	0 100 100	134, 175, 208, 229	0
3	V	8/8 (100%)	0.97	2 (25%) 1 1	171, 191, 238, 246	0
3	W	8/8 (100%)	1.38	2 (25%) 1 1	183, 213, 257, 277	0
3	X	8/8 (100%)	0.12	0 100 100	160, 200, 214, 221	0
3	Y	8/8 (100%)	0.39	1 (12%) 5 5	159, 207, 223, 255	0
3	Z	8/8 (100%)	0.56	1 (12%) 5 5	183, 210, 251, 254	0
All	All	1995/2169 (91%)	-0.38	36 (1%) 71 61	100, 182, 255, 336	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	711	GLY	4.7
1	C	697	ASN	4.3
1	B	419	ASN	4.3
1	C	510	GLN	3.6
3	W	361	TYR	3.5
1	D	697	ASN	3.5
1	F	712	GLU	3.5
1	C	711	GLY	3.2
1	F	492	GLU	3.1
1	C	421	SER	3.1
1	D	421	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	V	359	PRO	2.9
1	C	419	ASN	2.8
1	E	419	ASN	2.7
3	Z	355	ASP	2.6
1	F	711	GLY	2.6
1	C	683	VAL	2.6
3	W	360	GLU	2.5
1	D	419	ASN	2.5
1	F	446	LYS	2.5
1	E	709	PRO	2.5
1	D	510	GLN	2.4
1	B	421	SER	2.4
1	B	712	GLU	2.3
1	F	513	GLU	2.3
1	F	470	ASN	2.3
1	F	469	CYS	2.2
3	Y	361	TYR	2.2
1	B	513	GLU	2.2
1	C	480	SER	2.2
1	F	411	LEU	2.1
1	F	471	SER	2.1
1	B	420	GLY	2.1
1	E	418	TYR	2.1
1	F	594	VAL	2.1
3	V	361	TYR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.