



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:22 am BST

PDB ID : 4XF2
Title : Tetragonal structure of Arp2/3 complex
Authors : Jurgenson, C.T.; Pollard, T.P.
Deposited on : 2014-12-25
Resolution : 5.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

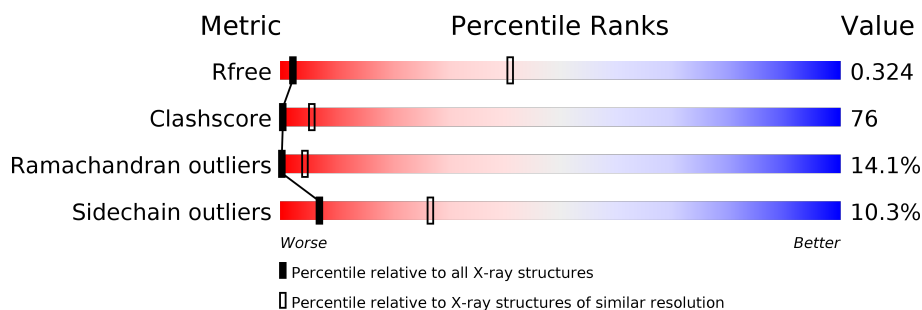
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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}	130704	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	418	24% 58% 11% • 6%
1	T	418	25% 56% 11% • 6%
2	B	394	22% 26% 9% • 42%
2	U	394	20% 28% 9% • 42%
3	C	372	19% 54% 20% • 5%
3	V	372	17% 57% 18% • 5%
4	D	300	28% 53% 13% • 5%

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Mol	Chain	Length	Quality of chain
4	W	300	<div><div></div><div>29%51%14%5%</div></div>
5	E	178	<div><div></div><div>26%62%10%</div></div>
5	X	178	<div><div></div><div>27%57%12%</div></div>
6	F	168	<div><div></div><div>29%58%12%</div></div>
6	Y	168	<div><div></div><div>24%59%15%</div></div>
7	G	151	<div><div></div><div>27%52%13%8%</div></div>
7	Z	151	<div><div></div><div>25%53%14%8%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27556 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3146	2022	522	587	15			
1	T	392	Total	C	N	O	S	0	0	0
			3146	2022	522	587	15			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	228	Total	C	N	O	S	0	0	0
			1734	1105	303	322	4			
2	U	228	Total	C	N	O	S	0	0	0
			1738	1108	304	322	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	354	Total	C	N	O	S	0	0	0
			2758	1747	487	505	19			
3	V	354	Total	C	N	O	S	0	0	0
			2758	1747	487	505	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	conflict	UNP Q58CQ2
V	58	VAL	ILE	conflict	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	284	Total	C	N	O	S	0	0	0
			2292	1456	397	431	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	284	Total	C	N	O	S	0	0	0
			2292	1456	397	431	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1415	908	236	262	9			
5	X	174	Total	C	N	O	S	0	0	0
			1415	908	236	262	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

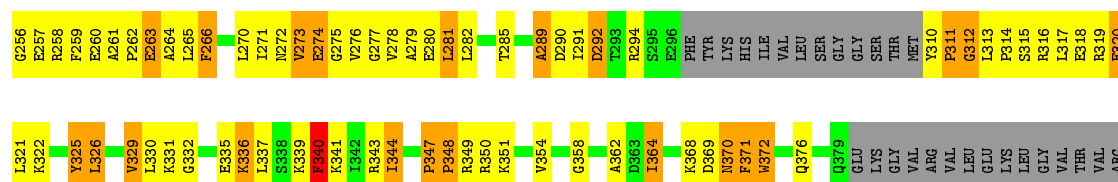
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			
6	Y	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	139	Total	C	N	O	S	0	0	0
			1060	661	185	211	3			
7	Z	139	Total	C	N	O	S	0	0	0
			1060	661	185	211	3			

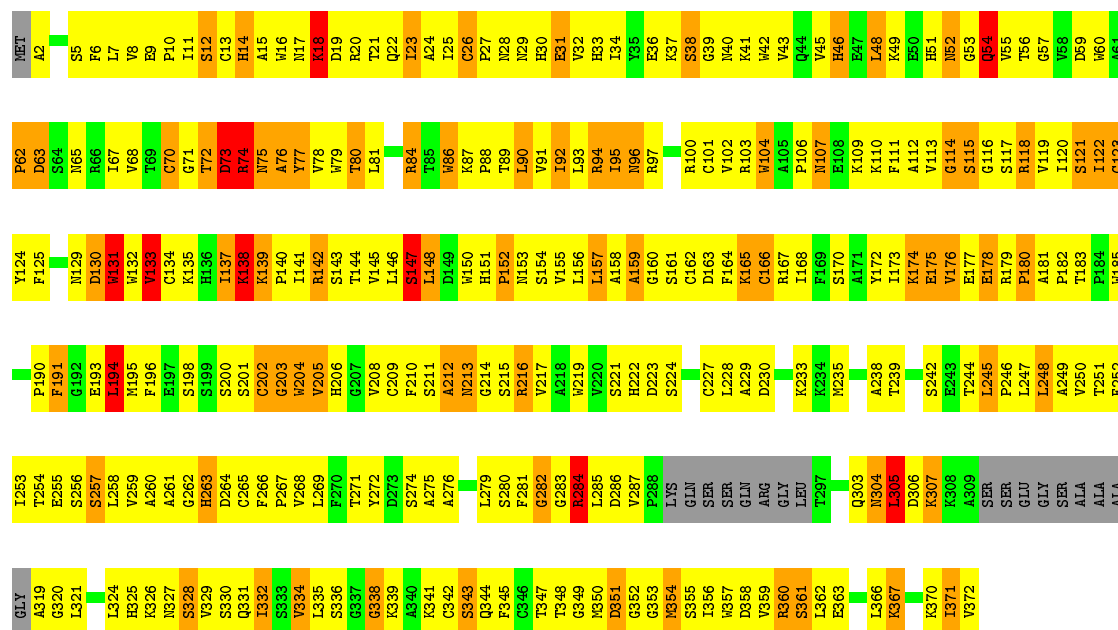
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	conflict	UNP Q3SYX9
G	28	ASP	GLU	conflict	UNP Q3SYX9
Z	17	ASP	GLY	conflict	UNP Q3SYX9
Z	28	ASP	GLU	conflict	UNP Q3SYX9



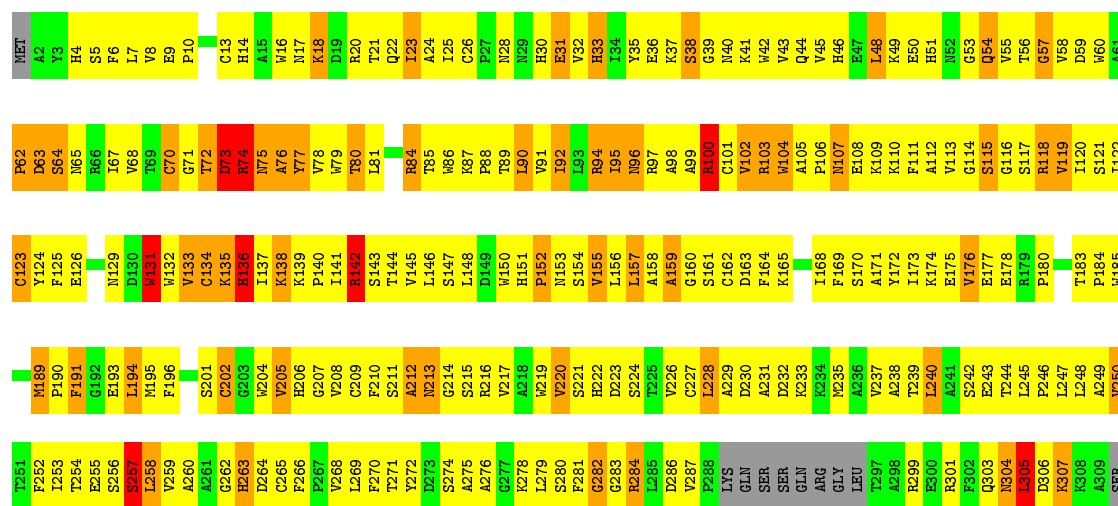
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

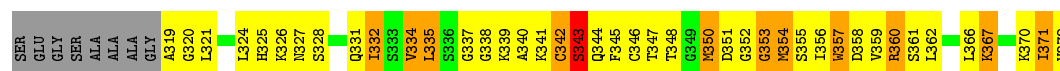
Chain C: 19% 54% 20% 5%



• Molecule 3: Actin-related protein 2/3 complex subunit 1B

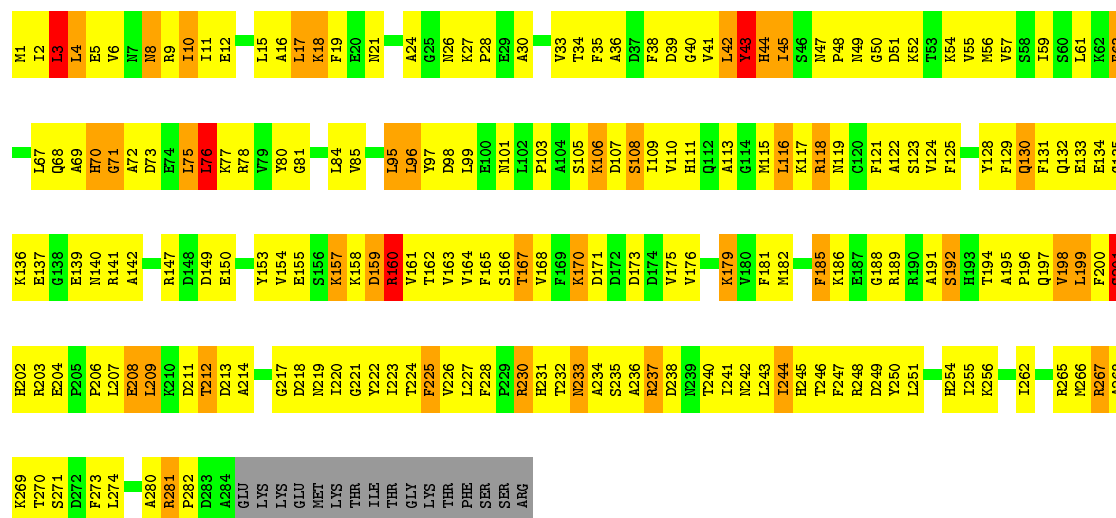
Chain V: 17% 57% 18% 5%





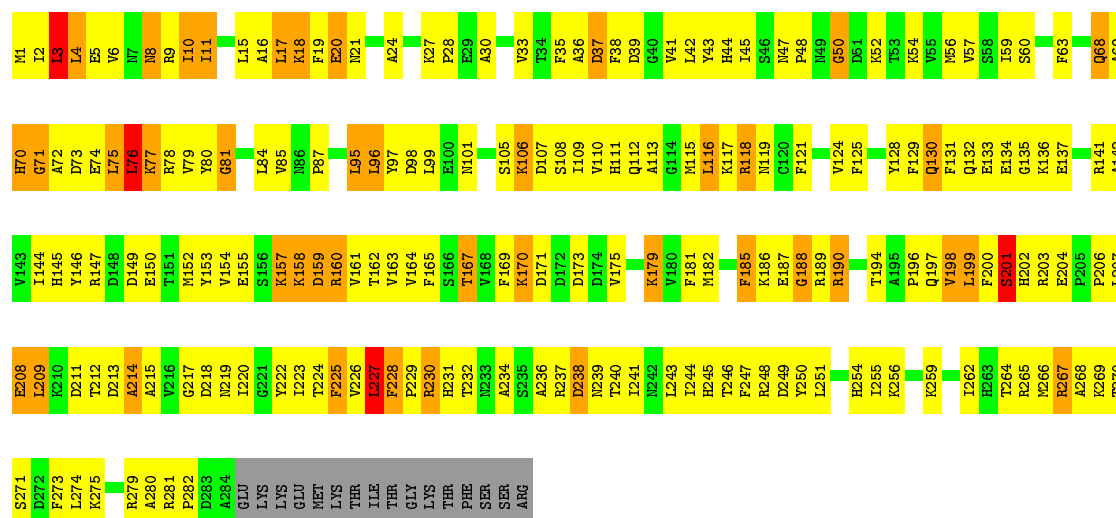
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D: 28% 53% 13% 5%



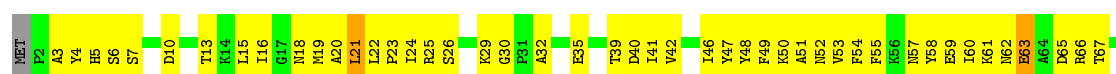
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain W: 29% 51% 14% 5%

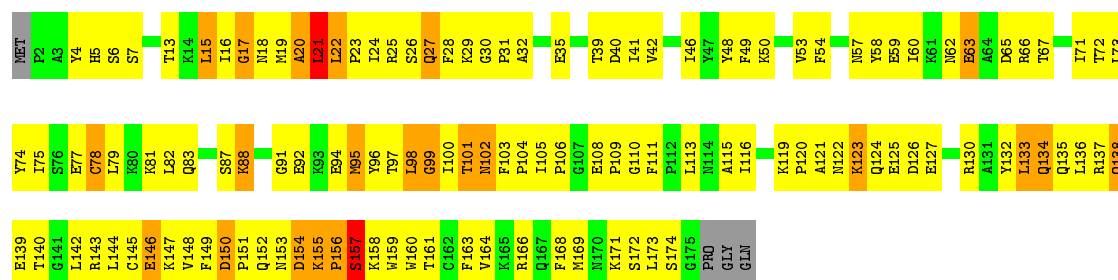


• Molecule 5: Actin-related protein 2/3 complex subunit 3

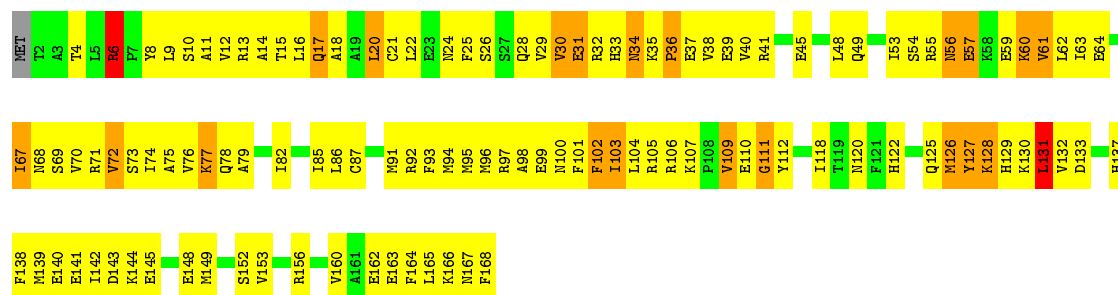
Chain E: 26% 62% 10% 5%



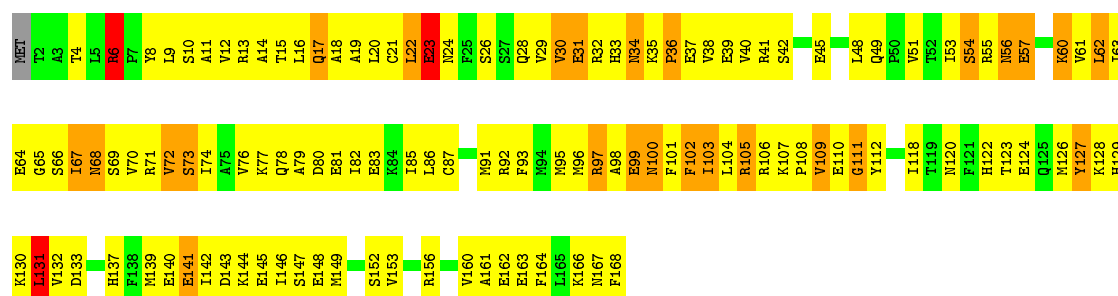
- Molecule 5: Actin-related protein 2/3 complex subunit 3



- Molecule 6: Actin-related protein 2/3 complex subunit 4

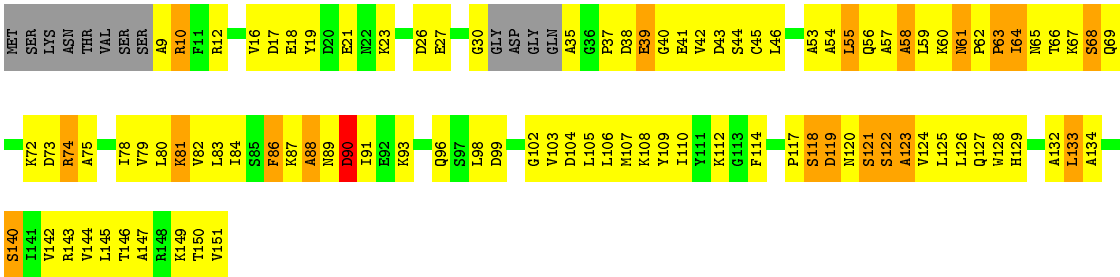


- Molecule 6: Actin-related protein 2/3 complex subunit 4

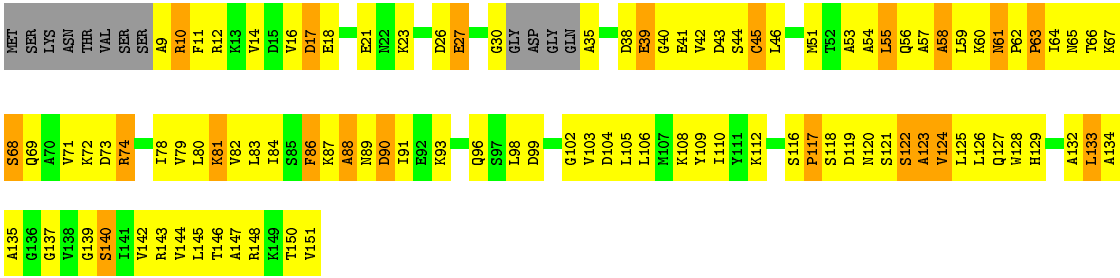


- Molecule 7: Actin-related protein 2/3 complex subunit 5





• Molecule 7: Actin-related protein 2/3 complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	149.93Å 149.93Å 265.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 5.00 47.54 – 4.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.54-5.00) 81.1 (47.54-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.275 , 0.303 0.311 , 0.324	Depositor DCC
R_{free} test set	1622 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	185.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 282.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	27556	wwPDB-VP
Average B, all atoms (Å ²)	256.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

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	0.42	0/3226	0.83	4/4376 (0.1%)
1	T	0.33	0/3226	0.64	2/4376 (0.0%)
2	B	0.40	0/1764	0.84	5/2389 (0.2%)
2	U	0.33	0/1768	0.67	4/2393 (0.2%)
3	C	0.35	0/2827	0.74	2/3832 (0.1%)
3	V	0.32	0/2827	0.62	0/3832
4	D	0.37	0/2341	0.72	2/3161 (0.1%)
4	W	0.33	0/2341	0.63	2/3161 (0.1%)
5	E	0.37	0/1449	0.71	0/1954
5	X	0.36	0/1449	0.65	0/1954
6	F	0.40	0/1393	0.80	1/1868 (0.1%)
6	Y	0.36	0/1393	0.73	1/1868 (0.1%)
7	G	0.33	0/1072	0.63	0/1442
7	Z	0.38	0/1072	0.67	0/1442
All	All	0.36	0/28148	0.71	23/38048 (0.1%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	LYS	C-N-CD	-9.01	100.78	120.60
4	D	267	ARG	NE-CZ-NH1	-6.56	117.02	120.30
4	D	96	LEU	CA-CB-CG	6.55	130.37	115.30
4	W	96	LEU	CA-CB-CG	6.54	130.35	115.30
6	Y	131	LEU	CA-CB-CG	6.50	130.24	115.30

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	3146	0	3089	442	0
1	T	3146	0	3087	561	0
2	B	1734	0	1641	156	0
2	U	1738	0	1653	224	0
3	C	2758	0	2713	539	0
3	V	2758	0	2711	609	0
4	D	2292	0	2257	444	2
4	W	2292	0	2257	391	1
5	E	1415	0	1416	181	1
5	X	1415	0	1416	230	2
6	F	1371	0	1410	202	0
6	Y	1371	0	1410	257	0
7	G	1060	0	1065	114	0
7	Z	1060	0	1065	119	0
All	All	27556	0	27190	4138	3

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 76.

The worst 5 of 4138 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:T:193:ILE:HG23	1:T:292:PHE:CE1	1.28	1.67
4:D:165:PHE:CZ	4:D:247:PHE:CE2	1.77	1.67
1:T:194:PRO:HD2	1:T:292:PHE:CE1	1.29	1.64
3:V:99:ALA:HA	3:V:115:SER:CB	1.19	1.59
2:B:202:TYR:CE2	2:B:252:ILE:HB	1.11	1.57

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:PHE:O	5:X:88:LYS:NZ[3_555]	1.85	0.35
5:E:88:LYS:NZ	4:W:200:PHE:O[3_545]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:LEU:CD2	5:X:146:GLU:OE1[3_555]	2.10	0.10

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	384/418 (92%)	270 (70%)	66 (17%)	48 (12%)	0	5
1	T	384/418 (92%)	264 (69%)	69 (18%)	51 (13%)	0	4
2	B	222/394 (56%)	139 (63%)	48 (22%)	35 (16%)	0	3
2	U	222/394 (56%)	132 (60%)	55 (25%)	35 (16%)	0	3
3	C	348/372 (94%)	207 (60%)	82 (24%)	59 (17%)	0	3
3	V	348/372 (94%)	208 (60%)	80 (23%)	60 (17%)	0	3
4	D	282/300 (94%)	189 (67%)	65 (23%)	28 (10%)	0	10
4	W	282/300 (94%)	186 (66%)	63 (22%)	33 (12%)	0	6
5	E	172/178 (97%)	124 (72%)	30 (17%)	18 (10%)	0	8
5	X	172/178 (97%)	116 (67%)	34 (20%)	22 (13%)	0	5
6	F	165/168 (98%)	120 (73%)	23 (14%)	22 (13%)	0	4
6	Y	165/168 (98%)	113 (68%)	29 (18%)	23 (14%)	0	4
7	G	135/151 (89%)	91 (67%)	21 (16%)	23 (17%)	0	3
7	Z	135/151 (89%)	84 (62%)	27 (20%)	24 (18%)	0	3
All	All	3416/3962 (86%)	2243 (66%)	692 (20%)	481 (14%)	0	4

5 of 481 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	28	GLN
1	A	150	ALA

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Mol	Chain	Res	Type
1	A	181	ALA
1	A	232	SER

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	345/363 (95%)	321 (93%)	24 (7%)	15	41
1	T	345/363 (95%)	319 (92%)	26 (8%)	13	39
2	B	168/345 (49%)	144 (86%)	24 (14%)	3	17
2	U	169/345 (49%)	147 (87%)	22 (13%)	4	20
3	C	301/313 (96%)	257 (85%)	44 (15%)	3	17
3	V	301/313 (96%)	264 (88%)	37 (12%)	4	21
4	D	249/264 (94%)	223 (90%)	26 (10%)	7	26
4	W	249/264 (94%)	225 (90%)	24 (10%)	8	29
5	E	156/159 (98%)	142 (91%)	14 (9%)	9	32
5	X	156/159 (98%)	136 (87%)	20 (13%)	4	20
6	F	154/155 (99%)	145 (94%)	9 (6%)	20	46
6	Y	154/155 (99%)	138 (90%)	16 (10%)	7	26
7	G	114/124 (92%)	103 (90%)	11 (10%)	8	29
7	Z	114/124 (92%)	105 (92%)	9 (8%)	12	38
All	All	2975/3446 (86%)	2669 (90%)	306 (10%)	7	27

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	131	LEU
1	T	294	GLN
6	Y	22	LEU
7	G	39	GLU
1	T	71	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	138	GLN
7	G	129	HIS
5	X	18	ASN
6	F	78	GLN
6	F	129	HIS

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.