



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:39 am GMT

PDB ID : 1V7N
Title : Human Thrombopoietin Functional Domain Complexed To Neutralizing Antibody TN1 Fab
Authors : Feese, M.D.; Tamada, T.; Kato, Y.; Maeda, Y.; Hirose, M.; Matsukura, Y.; Shigematsu, H.; Kato, T.; Miyazaki, H.; Kuroki, R.
Deposited on : 2003-12-18
Resolution : 3.30 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

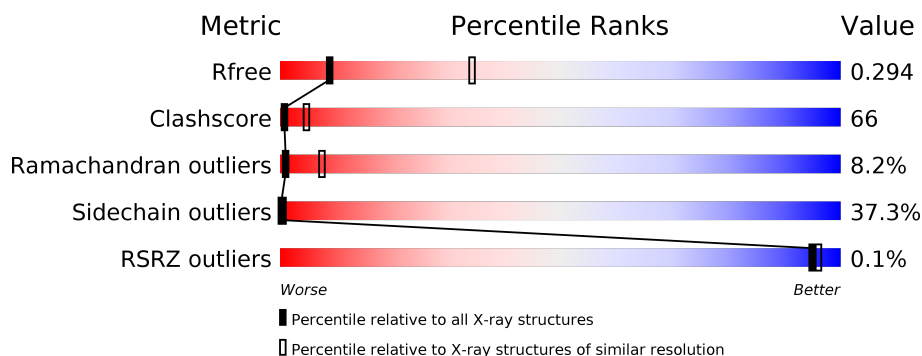
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	L	213	<div> <div>23%</div> <div>52%</div> <div>23%</div> <div>.</div> </div>
1	M	213	<div> <div>22%</div> <div>44%</div> <div>32%</div> <div>.</div> </div>
1	N	213	<div> <div>26%</div> <div>45%</div> <div>24%</div> <div>5%</div> </div>
1	O	213	<div> <div>20%</div> <div>51%</div> <div>27%</div> <div>.</div> </div>
2	H	217	<div> <div>25%</div> <div>48%</div> <div>20%</div> <div>7%</div> </div>
2	I	217	<div> <div>26%</div> <div>41%</div> <div>31%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	217	
2	K	217	
3	V	163	
3	X	163	
3	Y	163	
3	Z	163	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17466 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 Monoclonal TN1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1638	1018	278	333	9			
1	M	212	Total	C	N	O	S	0	0	0
			1632	1015	277	332	8			
1	N	212	Total	C	N	O	S	0	0	0
			1632	1015	277	332	8			
1	O	213	Total	C	N	O	S	0	0	0
			1638	1018	278	333	9			

- Molecule 2 is a protein called Monoclonal TN1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			
2	I	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			
2	J	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			
2	K	217	Total	C	N	O	S	0	0	0
			1630	1030	271	321	8			

- Molecule 3 is a protein called Thrombopoietin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	145	Total	C	N	O	S	0	0	0
			1090	694	194	195	7			
3	X	138	Total	C	N	O	S	0	0	0
			1049	671	187	186	5			
3	Y	139	Total	C	N	O	S	0	0	0
			1053	673	188	187	5			
3	Z	138	Total	C	N	O	S	0	0	0
			1045	669	187	184	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	115	ARG	GLN	ENGINEERED	UNP P40225
X	115	ARG	GLN	ENGINEERED	UNP P40225
Y	115	ARG	GLN	ENGINEERED	UNP P40225
Z	115	ARG	GLN	ENGINEERED	UNP P40225

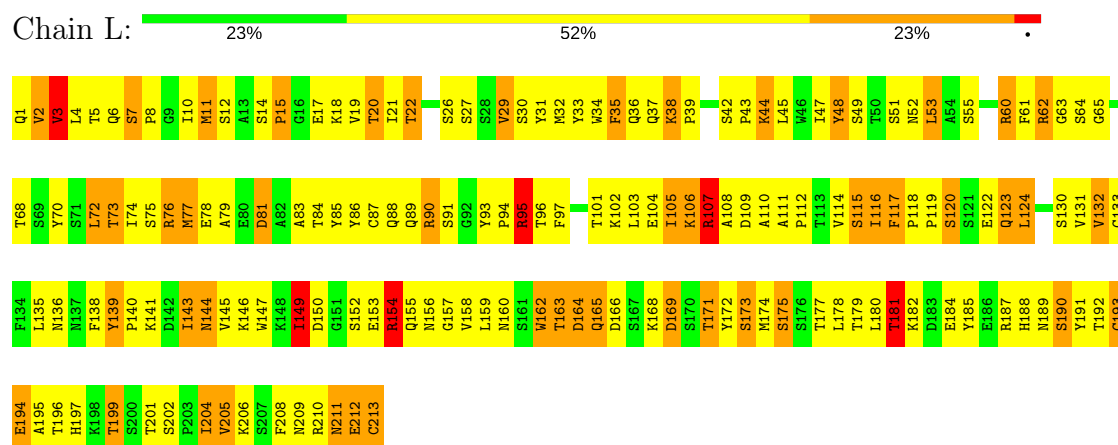
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	17	Total O 17 17	0	0
4	I	27	Total O 27 27	0	0
4	J	13	Total O 13 13	0	0
4	K	10	Total O 10 10	0	0
4	L	20	Total O 20 20	0	0
4	M	18	Total O 18 18	0	0
4	N	19	Total O 19 19	0	0
4	O	20	Total O 20 20	0	0
4	V	7	Total O 7 7	0	0
4	X	11	Total O 11 11	0	0
4	Y	3	Total O 3 3	0	0
4	Z	4	Total O 4 4	0	0

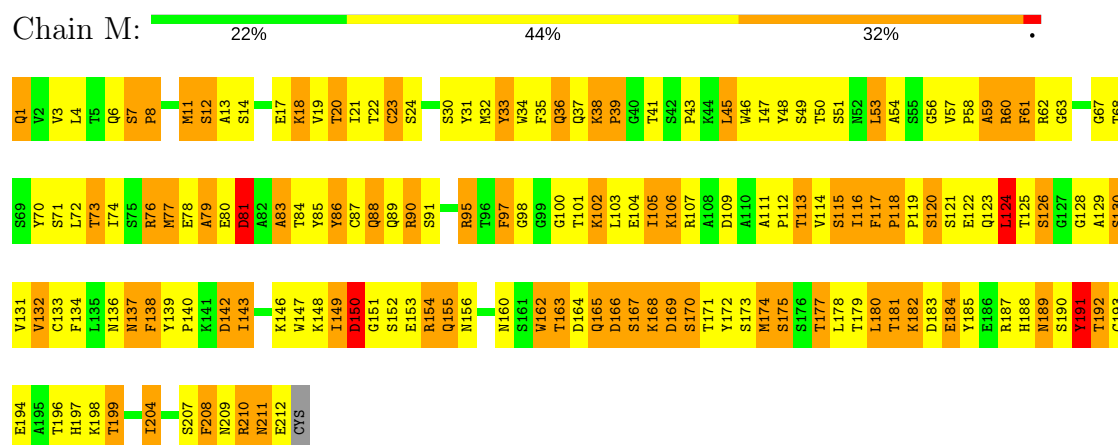
3 Residue-property plots

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

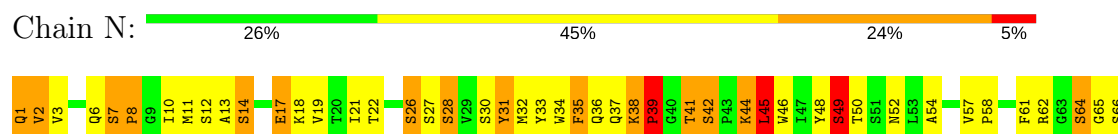
• Molecule 1: Monoclonal TN1 Fab Light Chain

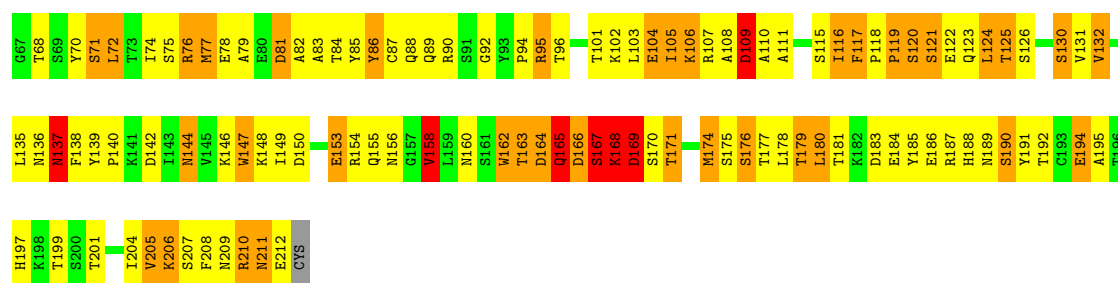


• Molecule 1: Monoclonal TN1 Fab Light Chain

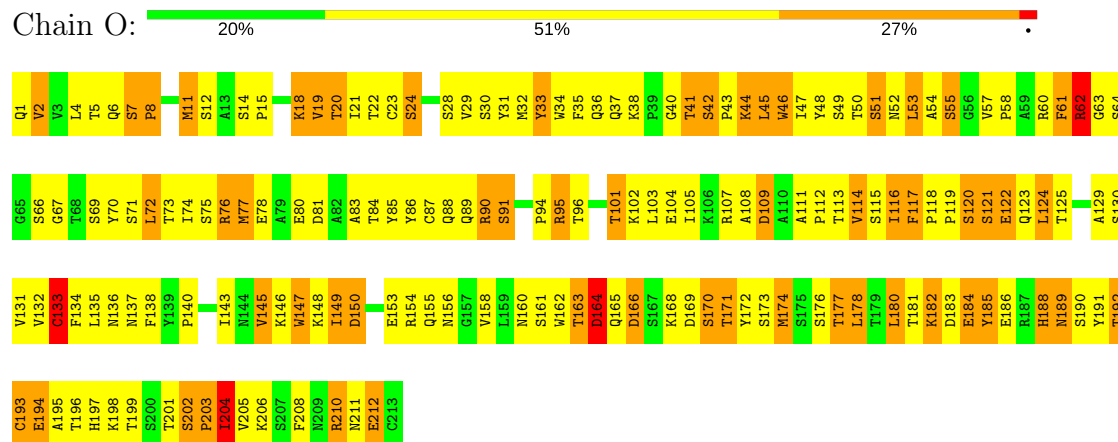


• Molecule 1: Monoclonal TN1 Fab Light Chain

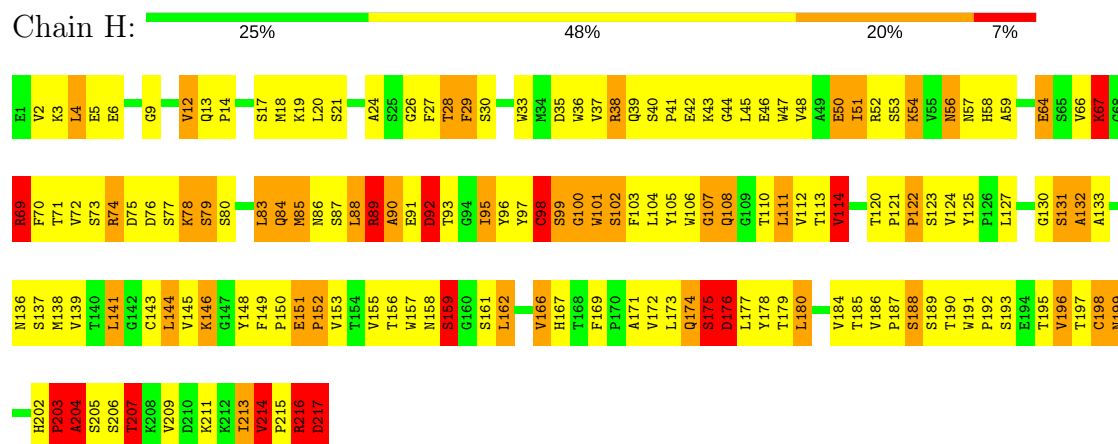




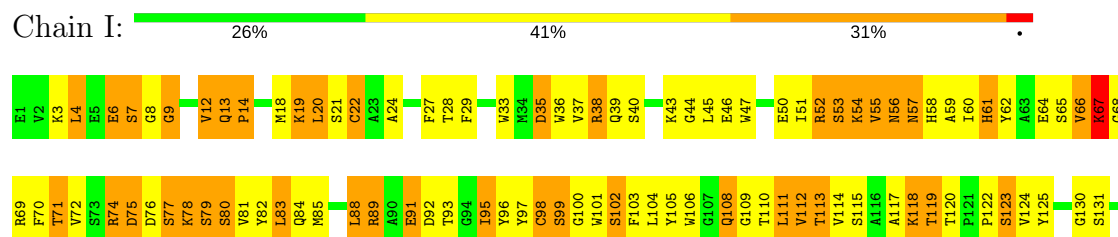
• Molecule 1: Monoclonal TN1 Fab Light Chain



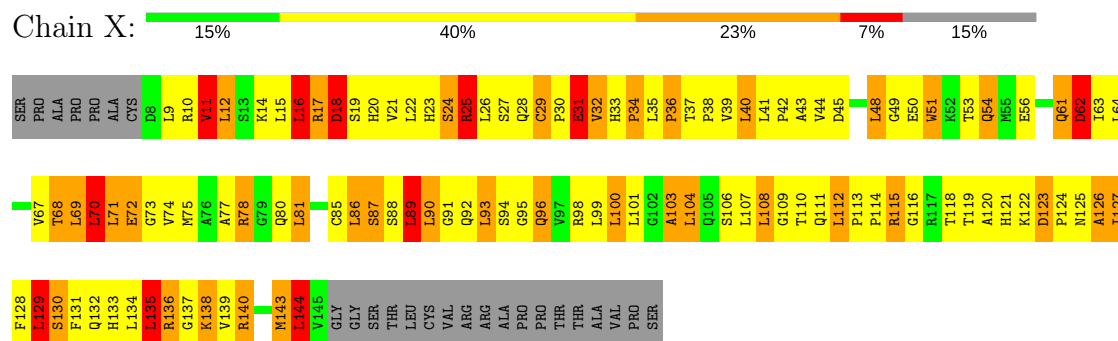
• Molecule 2: Monoclonal TN1 Fab Heavy Chain



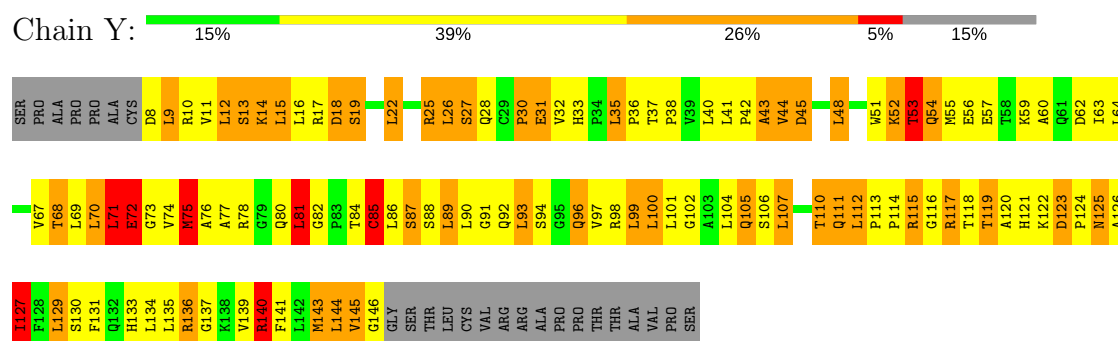
• Molecule 2: Monoclonal TN1 Fab Heavy Chain



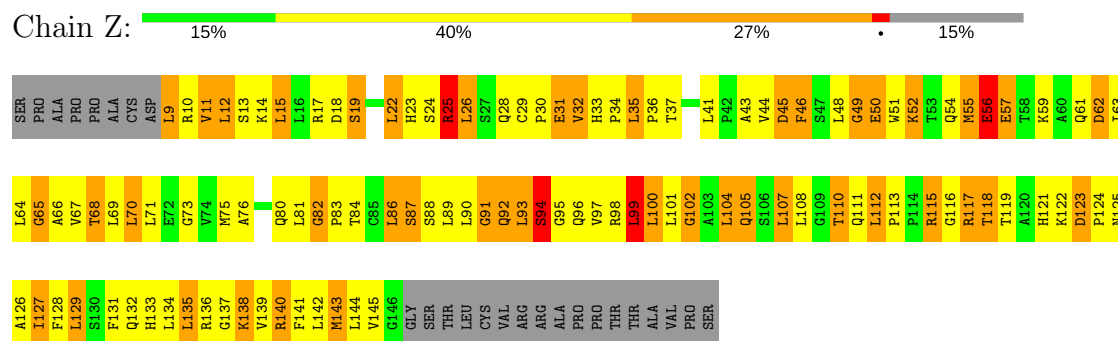
● Molecule 3: Thrombopoietin



● Molecule 3: Thrombopoietin



● Molecule 3: Thrombopoietin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.04Å 46.58Å 191.36Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	57.63 – 3.30 57.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (57.63-3.30) 98.4 (57.63-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.167 , 0.305 0.162 , 0.294	Depositor DCC
R_{free} test set	1801 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17466	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% 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	L	1.31	7/1676 (0.4%)	1.35	11/2274 (0.5%)
1	M	1.33	3/1670 (0.2%)	1.42	13/2266 (0.6%)
1	N	1.28	3/1670 (0.2%)	1.39	12/2266 (0.5%)
1	O	1.26	4/1676 (0.2%)	1.39	11/2274 (0.5%)
2	H	1.37	10/1674 (0.6%)	1.40	17/2289 (0.7%)
2	I	1.23	3/1674 (0.2%)	1.39	9/2289 (0.4%)
2	J	1.25	1/1674 (0.1%)	1.45	20/2289 (0.9%)
2	K	1.21	2/1674 (0.1%)	1.40	14/2289 (0.6%)
3	V	1.23	3/1109 (0.3%)	1.38	5/1506 (0.3%)
3	X	1.14	1/1068 (0.1%)	1.37	13/1451 (0.9%)
3	Y	1.24	2/1072 (0.2%)	1.48	15/1456 (1.0%)
3	Z	1.13	2/1064 (0.2%)	1.26	6/1445 (0.4%)
All	All	1.26	41/17701 (0.2%)	1.39	146/24094 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	2
1	N	0	2
2	H	0	2
2	I	0	5
2	J	0	3
2	K	0	2
3	X	0	1
3	Y	0	1
3	Z	0	2
All	All	0	20

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	139	TYR	CB-CG	-11.08	1.35	1.51
2	H	151	GLU	CD-OE2	8.63	1.35	1.25
1	L	48	TYR	CD2-CE2	-7.57	1.27	1.39
2	J	143	CYS	CB-SG	-7.46	1.69	1.82
2	H	98	CYS	CB-SG	-7.02	1.70	1.82

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	53	LEU	CA-CB-CG	-11.11	89.75	115.30
1	M	169	ASP	CB-CG-OD2	10.62	127.85	118.30
3	X	140	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	N	109	ASP	CB-CG-OD2	9.86	127.17	118.30
1	N	81	ASP	CB-CG-OD2	9.80	127.12	118.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	27	PHE	Peptide
2	H	99	SER	Peptide
2	I	7	SER	Peptide
1	M	61	PHE	Peptide
1	M	83	ALA	Peptide

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	L	1638	0	1573	218	1
1	M	1632	0	1568	247	0
1	N	1632	0	1568	213	0
1	O	1638	0	1573	216	0
2	H	1630	0	1568	220	0
2	I	1630	0	1568	194	0
2	J	1630	0	1568	231	0
2	K	1630	0	1568	240	0
3	V	1090	0	1135	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	1049	0	1098	157	0
3	Y	1053	0	1101	160	0
3	Z	1045	0	1097	143	0
4	H	17	0	0	9	0
4	I	27	0	0	4	0
4	J	13	0	0	2	0
4	K	10	0	0	5	0
4	L	20	0	0	3	0
4	M	18	0	0	5	0
4	N	19	0	0	2	0
4	O	20	0	0	5	0
4	V	7	0	0	0	1
4	X	11	0	0	5	0
4	Y	3	0	0	0	0
4	Z	4	0	0	0	0
All	All	17466	0	16985	2256	1

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 66.

The worst 5 of 2256 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:N:11:MET:SD	1:N:11:MET:CE	2.03	1.46
1:L:11:MET:CE	1:L:11:MET:SD	2.04	1.45
2:J:85:MET:CE	2:J:96:TYR:HE1	1.26	1.45
2:J:148:TYR:CE1	2:J:178:TYR:HB3	1.50	1.45
3:Z:55:MET:SD	3:Z:55:MET:CE	2.04	1.44

All (1) 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)
1:L:62:ARG:NH2	4:V:165:HOH:O[1_545]	2.19	0.01

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	L	211/213 (99%)	178 (84%)	28 (13%)	5 (2%)	7	35
1	M	210/213 (99%)	179 (85%)	20 (10%)	11 (5%)	2	16
1	N	210/213 (99%)	177 (84%)	20 (10%)	13 (6%)	2	13
1	O	211/213 (99%)	175 (83%)	24 (11%)	12 (6%)	2	14
2	H	215/217 (99%)	175 (81%)	24 (11%)	16 (7%)	1	9
2	I	215/217 (99%)	170 (79%)	25 (12%)	20 (9%)	1	5
2	J	215/217 (99%)	166 (77%)	31 (14%)	18 (8%)	1	7
2	K	215/217 (99%)	165 (77%)	30 (14%)	20 (9%)	1	5
3	V	143/163 (88%)	88 (62%)	32 (22%)	23 (16%)	0	1
3	X	136/163 (83%)	98 (72%)	19 (14%)	19 (14%)	0	1
3	Y	137/163 (84%)	92 (67%)	33 (24%)	12 (9%)	1	6
3	Z	136/163 (83%)	89 (65%)	31 (23%)	16 (12%)	0	2
All	All	2254/2372 (95%)	1752 (78%)	317 (14%)	185 (8%)	1	7

5 of 185 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	107	ARG
1	L	212	GLU
2	H	28	THR
2	H	133	ALA

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	L	186/186 (100%)	121 (65%)	65 (35%)	0	1
1	M	185/186 (100%)	118 (64%)	67 (36%)	0	1
1	N	185/186 (100%)	121 (65%)	64 (35%)	0	1
1	O	186/186 (100%)	117 (63%)	69 (37%)	0	0
2	H	182/185 (98%)	115 (63%)	67 (37%)	0	0
2	I	182/185 (98%)	108 (59%)	74 (41%)	0	0
2	J	182/185 (98%)	109 (60%)	73 (40%)	0	0
2	K	182/185 (98%)	115 (63%)	67 (37%)	0	0
3	V	122/138 (88%)	73 (60%)	49 (40%)	0	0
3	X	117/138 (85%)	74 (63%)	43 (37%)	0	0
3	Y	117/138 (85%)	72 (62%)	45 (38%)	0	0
3	Z	116/138 (84%)	74 (64%)	42 (36%)	0	1
All	All	1942/2036 (95%)	1217 (63%)	725 (37%)	0	0

5 of 725 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	180	LEU
2	J	200	VAL
3	Y	106	SER
2	J	3	LYS
2	J	85	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	6	GLN
2	J	58	HIS
3	Y	133	HIS
1	N	36	GLN
1	N	89	GLN

5.3.3 RNA ⓘ

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 [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	L	213/213 (100%)	-0.83	0 100 100	5, 23, 37, 46	0
1	M	212/213 (99%)	-0.74	0 100 100	5, 25, 40, 46	0
1	N	212/213 (99%)	-0.74	0 100 100	8, 26, 41, 49	0
1	O	213/213 (100%)	-0.69	0 100 100	7, 29, 50, 73	0
2	H	217/217 (100%)	-0.83	0 100 100	5, 23, 38, 63	0
2	I	217/217 (100%)	-0.78	0 100 100	10, 27, 44, 52	0
2	J	217/217 (100%)	-0.79	0 100 100	8, 24, 46, 67	0
2	K	217/217 (100%)	-0.60	0 100 100	13, 34, 54, 63	0
3	V	145/163 (88%)	-0.46	2 (1%) 75 73	8, 38, 81, 88	0
3	X	138/163 (84%)	-0.59	0 100 100	9, 32, 74, 83	0
3	Y	139/163 (85%)	-0.67	0 100 100	8, 27, 63, 70	0
3	Z	138/163 (84%)	-0.47	0 100 100	8, 41, 65, 77	0
All	All	2278/2372 (96%)	-0.70	2 (0%) 95 96	5, 27, 56, 88	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	7	CYS	4.3
3	V	151	CYS	2.7

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.