



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:35 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 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/ValidationPDFNotes.html>

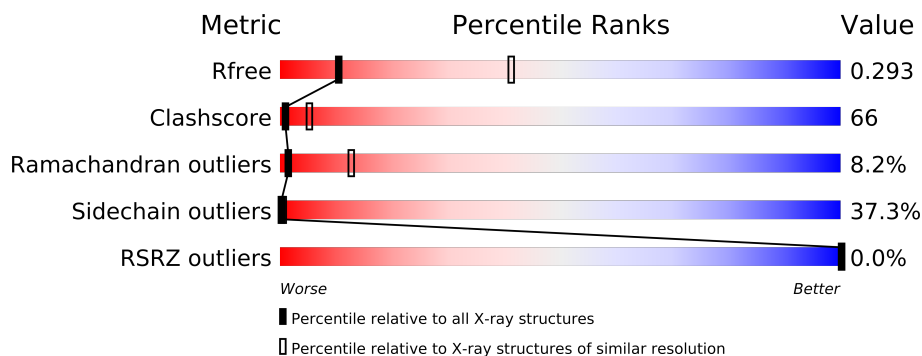
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	213	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	M	213	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	N	213	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	O	213	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	H	217	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	I	217	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	J	217	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	K	217	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	V	163	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	X	163	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	Y	163	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	Z	163	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17466 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

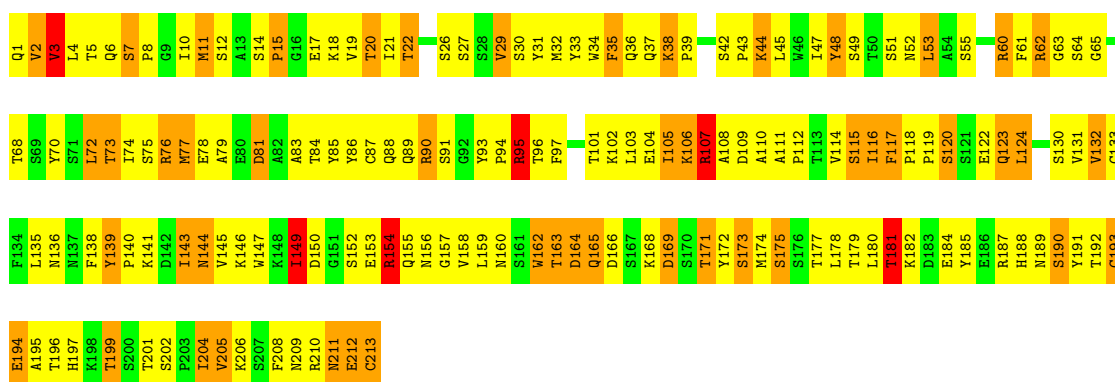
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	17	Total O 17 17	0	0
4	I	27	Total O 27 27	0	0
4	J	13	Total O 13 13	0	0
4	K	10	Total O 10 10	0	0
4	L	20	Total O 20 20	0	0
4	M	18	Total O 18 18	0	0
4	N	19	Total O 19 19	0	0
4	O	20	Total O 20 20	0	0
4	V	7	Total O 7 7	0	0
4	X	11	Total O 11 11	0	0
4	Y	3	Total O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

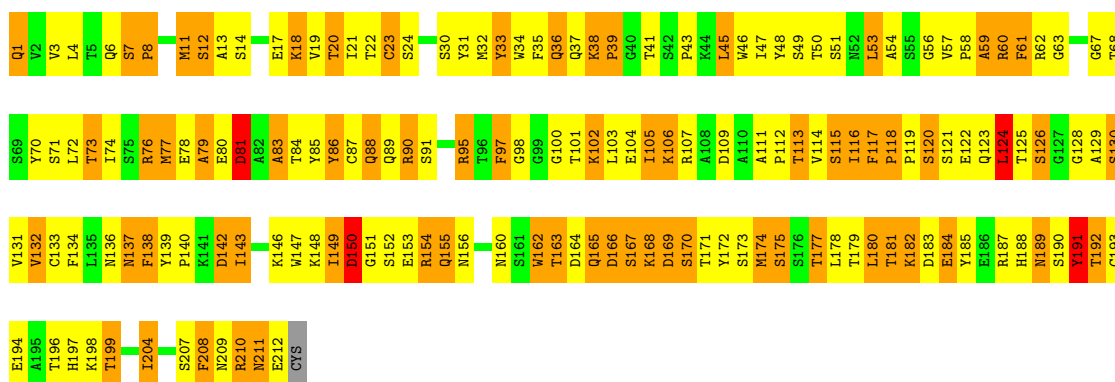
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain L:



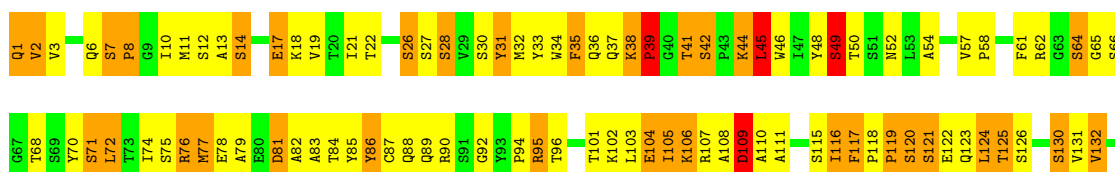
• Molecule 1: Monoclonal TN1 Fab Light Chain

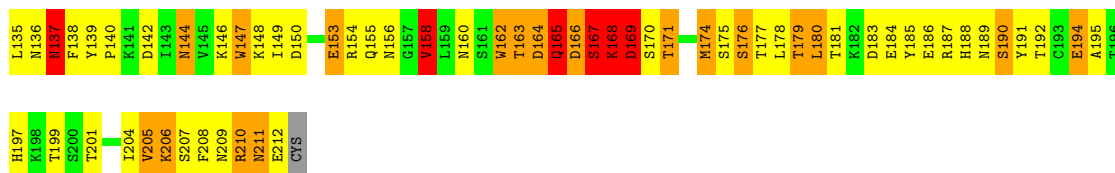
Chain M:



• Molecule 1: Monoclonal TN1 Fab Light Chain

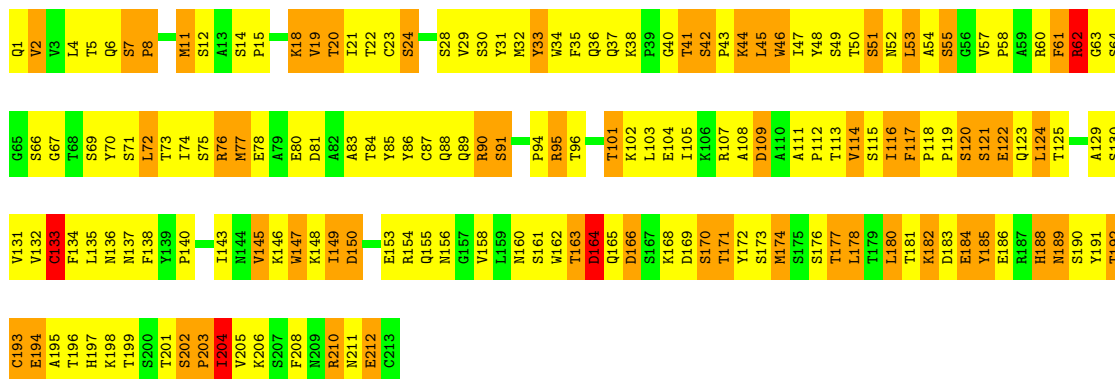
Chain N:





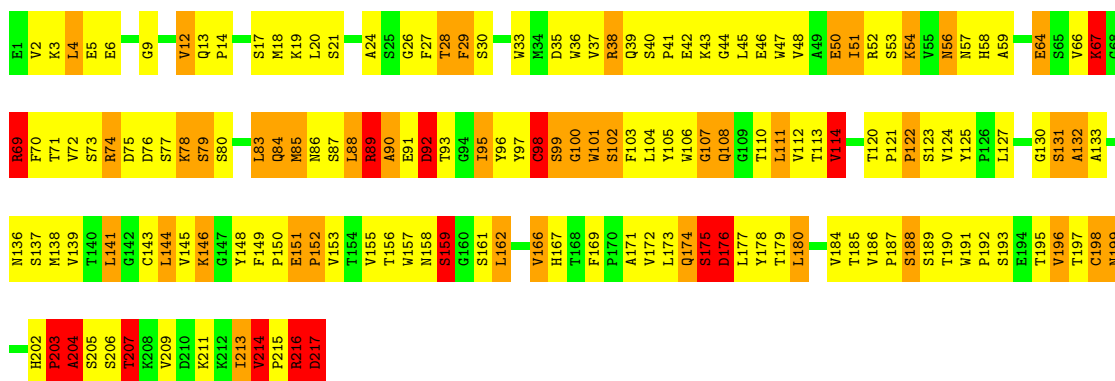
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain O:



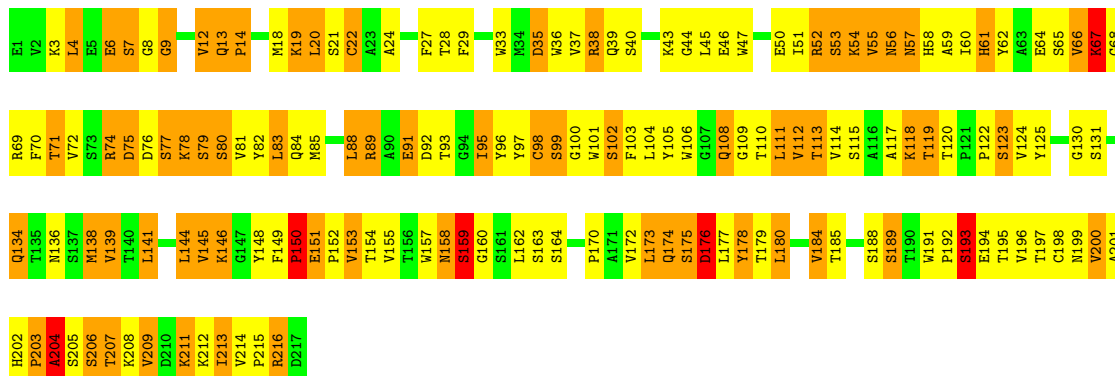
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain H:



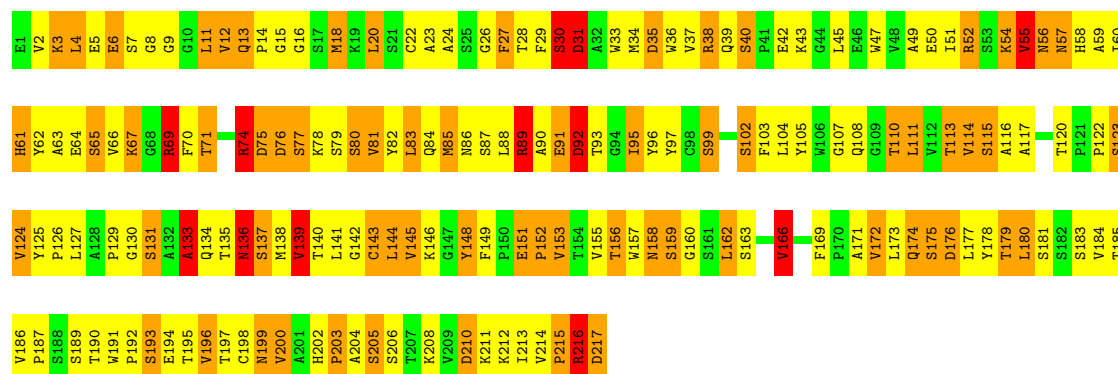
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain I:



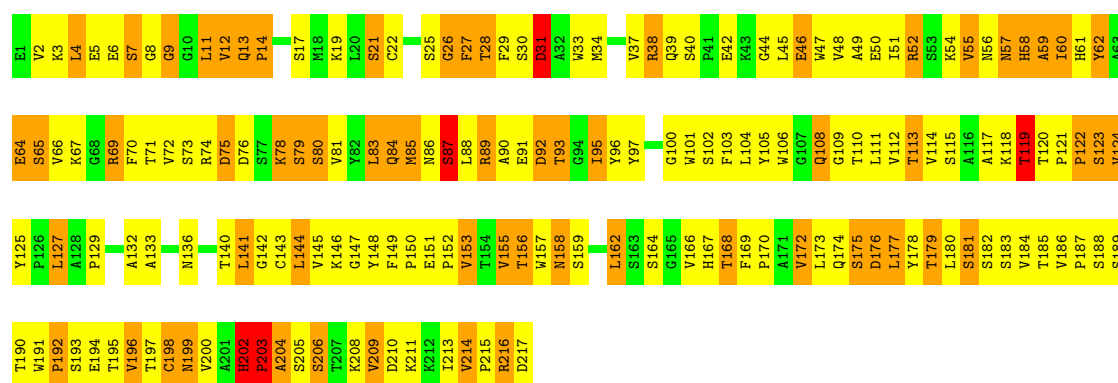
- Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain J:



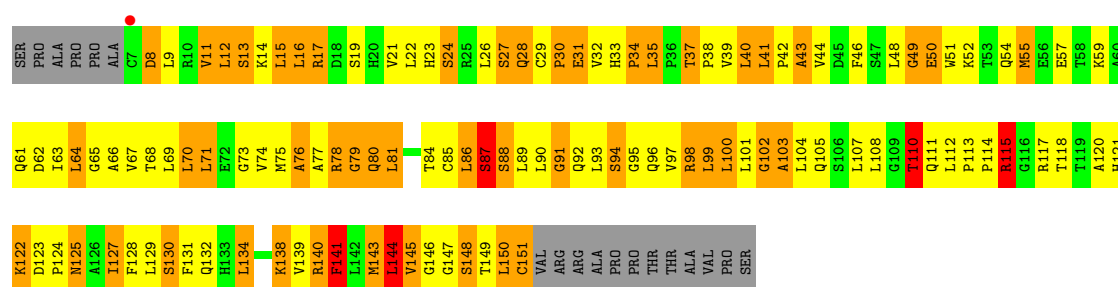
- Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain K:



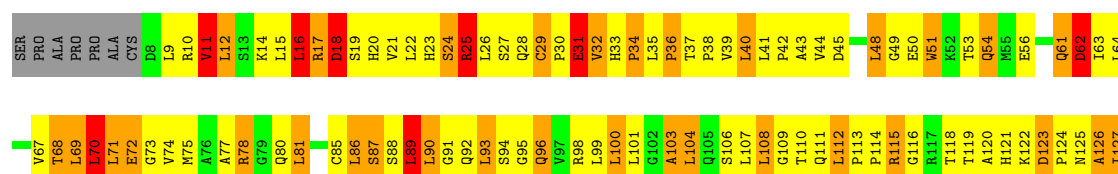
- Molecule 3: Thrombopoietin

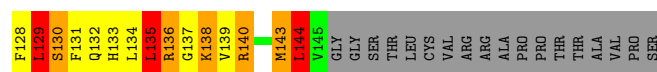
Chain V:



- Molecule 3: Thrombopoietin

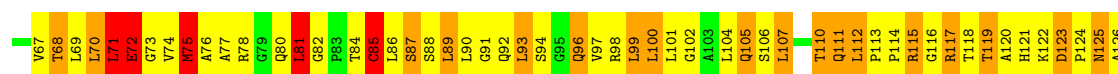
Chain X:





• Molecule 3: Thrombopoietin

Chain Y:



• Molecule 3: Thrombopoietin

Chain Z:



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 0.163 , 0.293	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)	0.27 , 34.0	EDS
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 35816 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1630	0	1568	240	0
3	V	1090	0	1135	153	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 66.

The worst 5 of 2256 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(Å)
1:L:62:ARG:NH2	4:V:165:HOH:O[1_545]	2.19	0.01

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	L	211/213 (99%)	178 (84%)	28 (13%)	5 (2%)	9	53
1	M	210/213 (99%)	179 (85%)	20 (10%)	11 (5%)	3	27
1	N	210/213 (99%)	177 (84%)	20 (10%)	13 (6%)	2	21
1	O	211/213 (99%)	175 (83%)	24 (11%)	12 (6%)	3	24
2	H	215/217 (99%)	175 (81%)	24 (11%)	16 (7%)	2	15
2	I	215/217 (99%)	170 (79%)	25 (12%)	20 (9%)	1	9
2	J	215/217 (99%)	166 (77%)	31 (14%)	18 (8%)	1	12
2	K	215/217 (99%)	165 (77%)	30 (14%)	20 (9%)	1	9
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	2
3	Y	137/163 (84%)	92 (67%)	33 (24%)	12 (9%)	1	11
3	Z	136/163 (83%)	89 (65%)	31 (23%)	16 (12%)	1	4
All	All	2254/2372 (95%)	1752 (78%)	317 (14%)	185 (8%)	1	13

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 ⓘ

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	1
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	1
3	V	122/138 (88%)	73 (60%)	49 (40%)	0	0
3	X	117/138 (85%)	74 (63%)	43 (37%)	0	1
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 chains 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 carbohydrates 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, 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%)	-0.53	0 100 100	5, 23, 37, 46	0
1	M	212/213 (99%)	-0.51	0 100 100	5, 25, 40, 46	0
1	N	212/213 (99%)	-0.51	0 100 100	8, 26, 41, 49	0
1	O	213/213 (100%)	-0.45	0 100 100	7, 29, 50, 73	0
2	H	217/217 (100%)	-0.53	0 100 100	5, 23, 38, 63	0
2	I	217/217 (100%)	-0.49	0 100 100	10, 27, 44, 52	0
2	J	217/217 (100%)	-0.49	0 100 100	8, 24, 46, 67	0
2	K	217/217 (100%)	-0.39	0 100 100	13, 34, 54, 63	0
3	V	145/163 (88%)	-0.32	1 (0%) 84 42	8, 38, 81, 88	0
3	X	138/163 (84%)	-0.40	0 100 100	9, 32, 74, 83	0
3	Y	139/163 (85%)	-0.44	0 100 100	8, 27, 63, 70	0
3	Z	138/163 (84%)	-0.34	0 100 100	8, 41, 65, 77	0
All	All	2278/2372 (96%)	-0.46	1 (0%) 100 100	5, 27, 56, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	7	CYS	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.