



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2019 – 10:28 PM EDT

PDB ID : 6E5U
Title : Crystal structure of the mRNA export receptor NXF1/NXT1 in complex with influenza virus NS1 protein
Authors : Xie, Y.; Ren, Y.
Deposited on : 2018-07-23
Resolution : 3.80 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	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

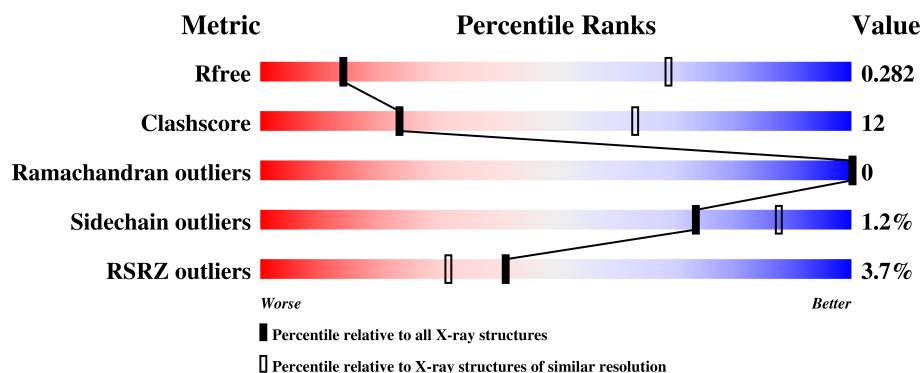
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)

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	508	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 49% 18% 33% </div> </div>
1	C	508	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 3% 49% 17% 33% </div> </div>
1	E	508	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 51% 15% 33% </div> </div>
1	G	508	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 49% 18% 33% </div> </div>
2	B	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 83% 16% . </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	140	
2	F	140	
2	H	140	
3	J	77	
3	K	77	
3	L	77	
3	M	77	
4	U	153	
4	V	153	
4	X	153	
4	Y	153	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20434 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 Nuclear RNA export factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2693	1702	469	512	10			
1	C	339	Total	C	N	O	S	0	0	0
			2693	1702	469	512	10			
1	E	339	Total	C	N	O	S	0	0	0
			2693	1702	469	512	10			
1	G	339	Total	C	N	O	S	0	0	0
			2693	1702	469	512	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	GLY	-	expression tag	UNP Q9UBU9
A	113	ALA	-	expression tag	UNP Q9UBU9
A	114	MET	-	expression tag	UNP Q9UBU9
A	115	GLY	-	expression tag	UNP Q9UBU9
C	112	GLY	-	expression tag	UNP Q9UBU9
C	113	ALA	-	expression tag	UNP Q9UBU9
C	114	MET	-	expression tag	UNP Q9UBU9
C	115	GLY	-	expression tag	UNP Q9UBU9
E	112	GLY	-	expression tag	UNP Q9UBU9
E	113	ALA	-	expression tag	UNP Q9UBU9
E	114	MET	-	expression tag	UNP Q9UBU9
E	115	GLY	-	expression tag	UNP Q9UBU9
G	112	GLY	-	expression tag	UNP Q9UBU9
G	113	ALA	-	expression tag	UNP Q9UBU9
G	114	MET	-	expression tag	UNP Q9UBU9
G	115	GLY	-	expression tag	UNP Q9UBU9

- Molecule 2 is a protein called NTF2-related export protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1099	693	185	214	7			
2	D	138	Total	C	N	O	S	0	0	0
			1099	693	185	214	7			
2	F	138	Total	C	N	O	S	0	0	0
			1099	693	185	214	7			
2	H	138	Total	C	N	O	S	0	0	0
			1099	693	185	214	7			

- Molecule 3 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	71	Total	C	N	O	S	0	0	0
			554	343	100	109	2			
3	L	38	Total	C	N	O	S	0	0	0
			307	194	56	56	1			
3	M	71	Total	C	N	O	S	0	0	0
			554	343	100	109	2			
3	J	38	Total	C	N	O	S	0	0	0
			307	194	56	56	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	GLY	-	expression tag	UNP I7CAR2
K	-3	ALA	-	expression tag	UNP I7CAR2
K	-2	MET	-	expression tag	UNP I7CAR2
K	-1	GLY	-	expression tag	UNP I7CAR2
K	0	SER	-	expression tag	UNP I7CAR2
K	38	ALA	ARG	engineered mutation	UNP I7CAR2
K	41	ALA	LYS	engineered mutation	UNP I7CAR2
L	-4	GLY	-	expression tag	UNP I7CAR2
L	-3	ALA	-	expression tag	UNP I7CAR2
L	-2	MET	-	expression tag	UNP I7CAR2
L	-1	GLY	-	expression tag	UNP I7CAR2
L	0	SER	-	expression tag	UNP I7CAR2
L	38	ALA	ARG	engineered mutation	UNP I7CAR2
L	41	ALA	LYS	engineered mutation	UNP I7CAR2
M	-4	GLY	-	expression tag	UNP I7CAR2
M	-3	ALA	-	expression tag	UNP I7CAR2
M	-2	MET	-	expression tag	UNP I7CAR2
M	-1	GLY	-	expression tag	UNP I7CAR2
M	0	SER	-	expression tag	UNP I7CAR2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	38	ALA	ARG	engineered mutation	UNP I7CAR2
M	41	ALA	LYS	engineered mutation	UNP I7CAR2
J	-4	GLY	-	expression tag	UNP I7CAR2
J	-3	ALA	-	expression tag	UNP I7CAR2
J	-2	MET	-	expression tag	UNP I7CAR2
J	-1	GLY	-	expression tag	UNP I7CAR2
J	0	SER	-	expression tag	UNP I7CAR2
J	38	ALA	ARG	engineered mutation	UNP I7CAR2
J	41	ALA	LYS	engineered mutation	UNP I7CAR2

- Molecule 4 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	115	Total	C	N	O	S	0	0	0
			909	578	154	170	7			
4	V	110	Total	C	N	O	S	0	0	0
			863	547	146	163	7			
4	X	115	Total	C	N	O	S	0	0	0
			909	578	154	170	7			
4	Y	110	Total	C	N	O	S	0	0	0
			863	547	146	163	7			

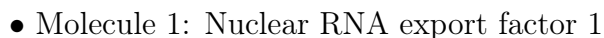
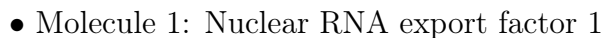
There are 24 discrepancies between the modelled and reference sequences:

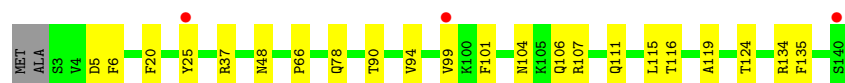
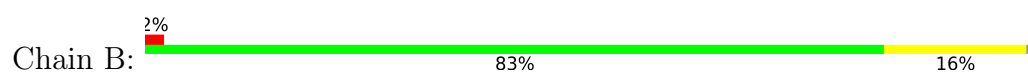
Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	THR	deletion	UNP I7CAR2
U	?	-	MET	deletion	UNP I7CAR2
U	?	-	ALA	deletion	UNP I7CAR2
U	?	-	SER	deletion	UNP I7CAR2
U	?	-	ALA	deletion	UNP I7CAR2
U	85	PRO	LEU	engineered mutation	UNP I7CAR2
V	?	-	THR	deletion	UNP I7CAR2
V	?	-	MET	deletion	UNP I7CAR2
V	?	-	ALA	deletion	UNP I7CAR2
V	?	-	SER	deletion	UNP I7CAR2
V	?	-	ALA	deletion	UNP I7CAR2
V	85	PRO	LEU	engineered mutation	UNP I7CAR2
X	?	-	THR	deletion	UNP I7CAR2
X	?	-	MET	deletion	UNP I7CAR2
X	?	-	ALA	deletion	UNP I7CAR2
X	?	-	SER	deletion	UNP I7CAR2
X	?	-	ALA	deletion	UNP I7CAR2

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Chain	Residue	Modelled	Actual	Comment	Reference
X	85	PRO	LEU	engineered mutation	UNP I7CAR2
Y	?	-	THR	deletion	UNP I7CAR2
Y	?	-	MET	deletion	UNP I7CAR2
Y	?	-	ALA	deletion	UNP I7CAR2
Y	?	-	SER	deletion	UNP I7CAR2
Y	?	-	ALA	deletion	UNP I7CAR2
Y	85	PRO	LEU	engineered mutation	UNP I7CAR2

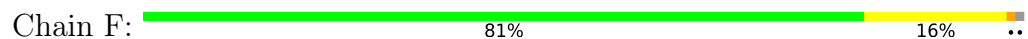




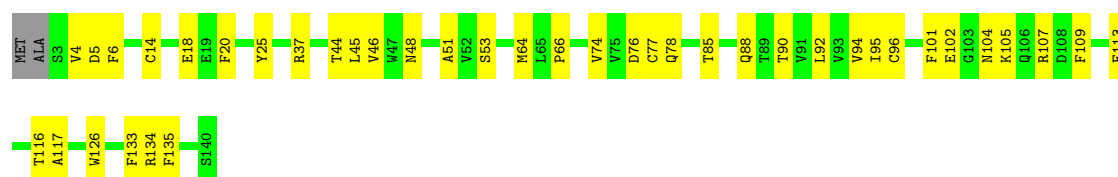
- Molecule 2: NTF2-related export protein 1



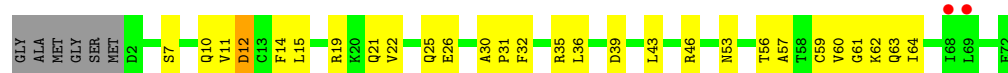
- Molecule 2: NTF2-related export protein 1



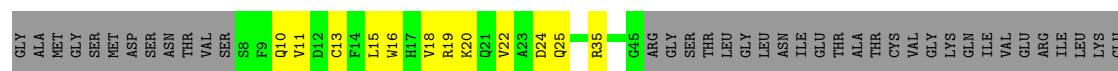
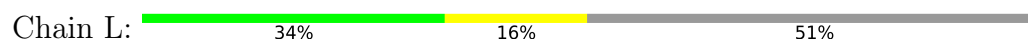
- Molecule 2: NTF2-related export protein 1



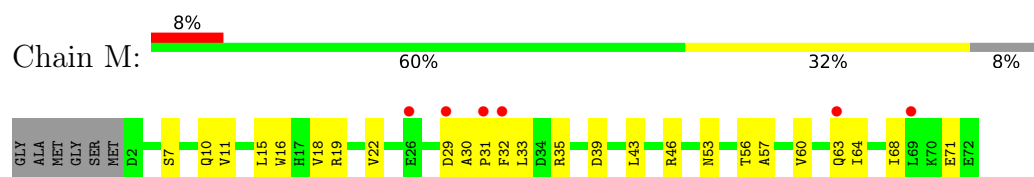
- Molecule 3: Non-structural protein 1



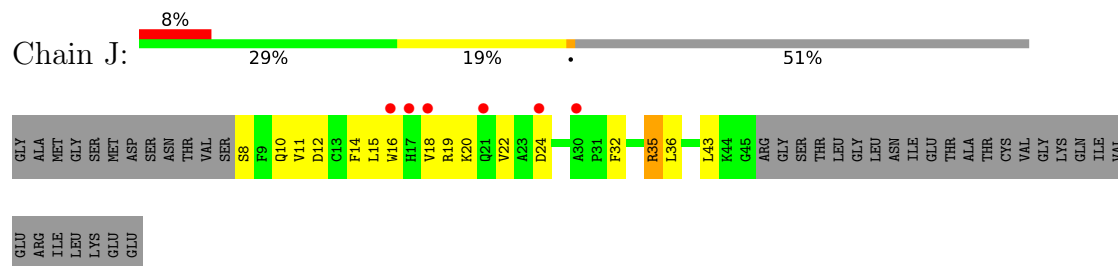
- Molecule 3: Non-structural protein 1



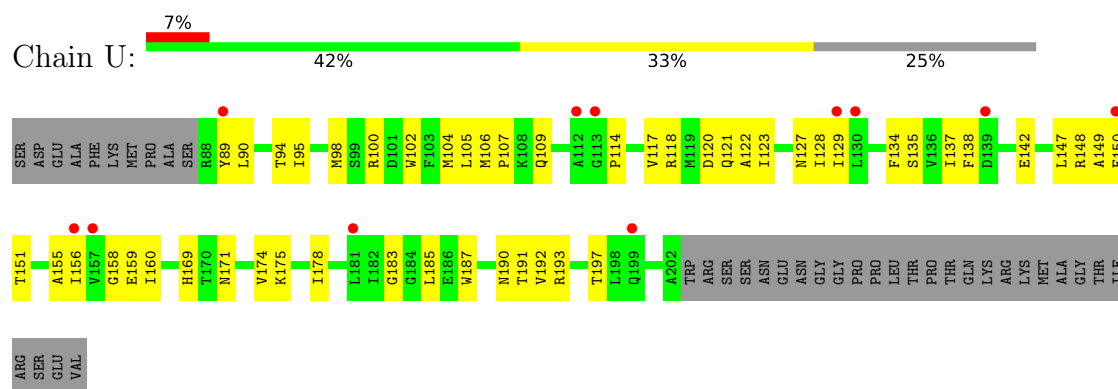
- Molecule 3: Non-structural protein 1



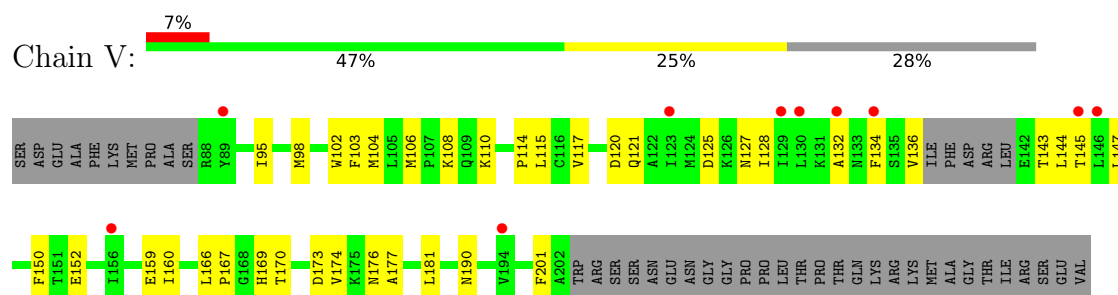
- Molecule 3: Non-structural protein 1



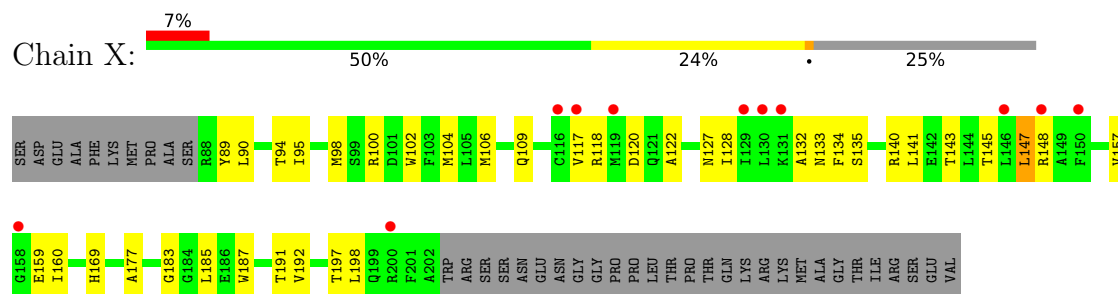
- Molecule 4: Non-structural protein 1



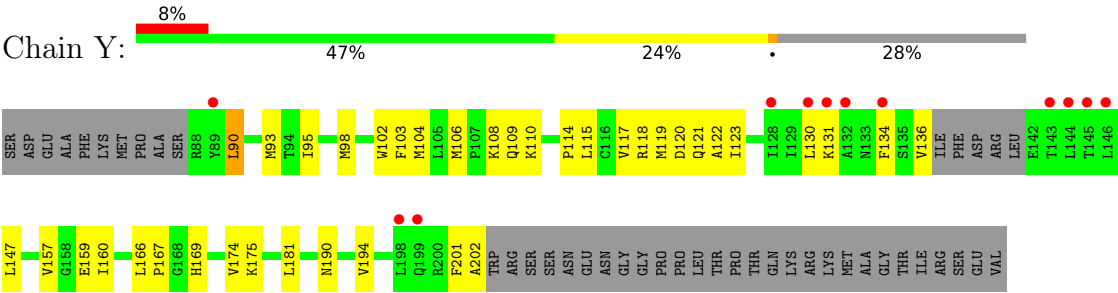
- Molecule 4: Non-structural protein 1



- Molecule 4: Non-structural protein 1



- Molecule 4: Non-structural protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	101.91Å 101.91Å 949.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.13 – 3.80 44.13 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.13-3.80) 98.5 (44.13-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.236 , 0.282 0.236 , 0.282	Depositor DCC
R_{free} test set	2135 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	141.8	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 187.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.420 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20434	wwPDB-VP
Average B, all atoms (Å ²)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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	0.31	0/2738	0.53	0/3699
1	C	0.32	0/2738	0.55	0/3699
1	E	0.31	0/2738	0.53	0/3699
1	G	0.33	0/2738	0.57	1/3699 (0.0%)
2	B	0.35	0/1123	0.54	0/1524
2	D	0.39	0/1123	0.56	0/1524
2	F	0.34	0/1123	0.53	0/1524
2	H	0.37	0/1123	0.55	0/1524
3	J	0.40	0/313	0.53	0/421
3	K	0.28	0/560	0.49	0/754
3	L	0.28	0/313	0.42	0/421
3	M	0.27	0/560	0.48	0/754
4	U	0.29	0/924	0.55	0/1250
4	V	0.29	0/876	0.57	0/1184
4	X	0.28	0/924	0.55	0/1250
4	Y	0.29	0/876	0.57	1/1184 (0.1%)
All	All	0.32	0/20790	0.54	2/28110 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	90	LEU	CA-CB-CG	5.15	127.14	115.30
1	G	369	THR	C-N-CA	5.12	134.49	121.70

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	2693	0	2724	58	0
1	C	2693	0	2724	67	0
1	E	2693	0	2724	51	0
1	G	2693	0	2724	71	0
2	B	1099	0	1050	16	0
2	D	1099	0	1050	32	0
2	F	1099	0	1050	21	0
2	H	1099	0	1050	34	0
3	J	307	0	296	17	0
3	K	554	0	551	23	0
3	L	307	0	296	10	0
3	M	554	0	551	26	0
4	U	909	0	923	38	0
4	V	863	0	874	32	0
4	X	909	0	923	30	0
4	Y	863	0	874	28	0
All	All	20434	0	20384	493	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 12.

The worst 5 of 493 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)
3:M:29:ASP:HB3	3:M:32:PHE:HB3	1.46	0.95
4:V:115:LEU:HD11	4:V:177:ALA:HB2	1.59	0.84
1:E:295:ILE:HG23	1:E:319:GLU:HB3	1.65	0.78
1:A:356:LEU:HD12	1:A:357:PRO:HD2	1.66	0.78
1:A:295:ILE:HG23	1:A:319:GLU:HB3	1.66	0.76

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	335/508 (66%)	319 (95%)	16 (5%)	0	100	100
1	C	335/508 (66%)	317 (95%)	18 (5%)	0	100	100
1	E	335/508 (66%)	320 (96%)	15 (4%)	0	100	100
1	G	335/508 (66%)	320 (96%)	15 (4%)	0	100	100
2	B	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
2	D	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
2	F	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
2	H	136/140 (97%)	134 (98%)	2 (2%)	0	100	100
3	J	36/77 (47%)	36 (100%)	0	0	100	100
3	K	69/77 (90%)	66 (96%)	3 (4%)	0	100	100
3	L	36/77 (47%)	36 (100%)	0	0	100	100
3	M	69/77 (90%)	68 (99%)	1 (1%)	0	100	100
4	U	113/153 (74%)	106 (94%)	7 (6%)	0	100	100
4	V	106/153 (69%)	103 (97%)	3 (3%)	0	100	100
4	X	113/153 (74%)	106 (94%)	7 (6%)	0	100	100
4	Y	106/153 (69%)	100 (94%)	6 (6%)	0	100	100
All	All	2532/3512 (72%)	2430 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	305/454 (67%)	301 (99%)	4 (1%)	71	87
1	C	305/454 (67%)	301 (99%)	4 (1%)	71	87
1	E	305/454 (67%)	302 (99%)	3 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	305/454 (67%)	300 (98%)	5 (2%)	65	85
2	B	123/124 (99%)	123 (100%)	0	100	100
2	D	123/124 (99%)	123 (100%)	0	100	100
2	F	123/124 (99%)	121 (98%)	2 (2%)	65	85
2	H	123/124 (99%)	122 (99%)	1 (1%)	83	92
3	J	32/64 (50%)	28 (88%)	4 (12%)	5	28
3	K	61/64 (95%)	60 (98%)	1 (2%)	65	85
3	L	32/64 (50%)	29 (91%)	3 (9%)	9	40
3	M	61/64 (95%)	61 (100%)	0	100	100
4	U	101/133 (76%)	101 (100%)	0	100	100
4	V	96/133 (72%)	96 (100%)	0	100	100
4	X	101/133 (76%)	100 (99%)	1 (1%)	78	89
4	Y	96/133 (72%)	96 (100%)	0	100	100
All	All	2292/3100 (74%)	2264 (99%)	28 (1%)	74	88

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	48	ASN
1	G	297	ASN
3	J	14	PHE
1	G	250	ARG
1	G	281	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	78	GLN
1	G	275	ASN
4	V	121	GLN
2	F	110	ASN
1	G	225	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	A	339/508 (66%)	-0.15	3 (0%) 84 77	111, 210, 335, 435	0
1	C	339/508 (66%)	0.06	16 (4%) 31 24	95, 185, 348, 440	0
1	E	339/508 (66%)	-0.12	5 (1%) 73 64	118, 206, 330, 416	0
1	G	339/508 (66%)	-0.02	9 (2%) 54 43	95, 180, 323, 417	0
2	B	138/140 (98%)	0.17	3 (2%) 62 51	117, 171, 244, 269	0
2	D	138/140 (98%)	-0.02	1 (0%) 87 82	101, 143, 245, 310	0
2	F	138/140 (98%)	0.06	0 100 100	106, 160, 225, 264	0
2	H	138/140 (98%)	0.03	0 100 100	104, 145, 246, 325	0
3	J	38/77 (49%)	0.42	6 (15%) 2 2	290, 387, 487, 545	0
3	K	71/77 (92%)	-0.43	2 (2%) 53 42	194, 261, 383, 401	0
3	L	38/77 (49%)	-0.45	0 100 100	248, 318, 419, 435	0
3	M	71/77 (92%)	0.09	6 (8%) 11 9	248, 306, 471, 529	0
4	U	115/153 (75%)	0.21	11 (9%) 8 6	193, 256, 338, 408	0
4	V	110/153 (71%)	0.38	10 (9%) 9 7	177, 307, 400, 487	0
4	X	115/153 (75%)	0.21	11 (9%) 8 6	192, 256, 341, 412	0
4	Y	110/153 (71%)	0.23	12 (10%) 5 5	162, 301, 378, 420	0
All	All	2576/3512 (73%)	0.02	95 (3%) 41 32	95, 209, 364, 545	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Y	144	LEU	9.1
4	V	130	LEU	9.0
4	V	194	VAL	8.4
4	V	89	TYR	7.5
4	Y	145	THR	6.3

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.