



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:27 am BST

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 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

<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

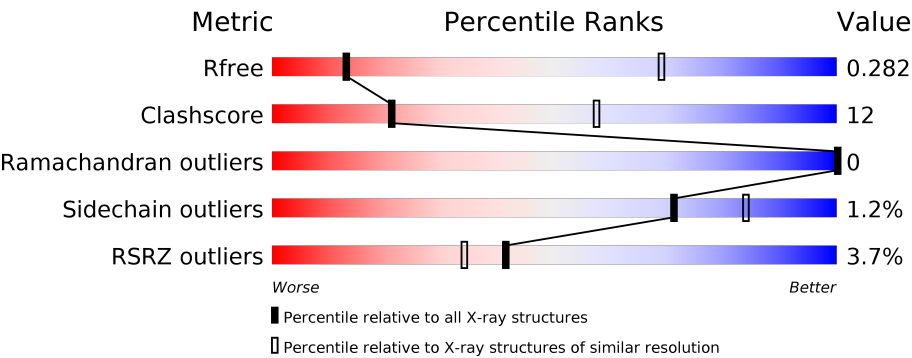
1 Overall quality at a glance i

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.









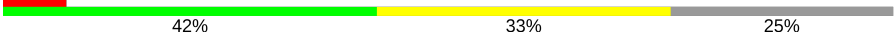
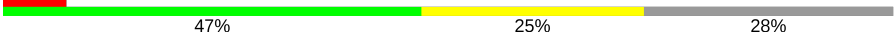

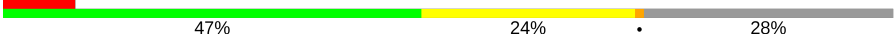
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 $\leq 5\%$. 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>%</div><div><div></div><div>49%</div><div>18%</div><div>33%</div></div></div>
1	C	508	<div><div>3%</div><div><div></div><div>49%</div><div>17%</div><div>33%</div></div></div>
1	E	508	<div><div>%</div><div><div></div><div>51%</div><div>15%</div><div>33%</div></div></div>
1	G	508	<div><div>2%</div><div><div></div><div>49%</div><div>18%</div><div>33%</div></div></div>
2	B	140	<div><div>2%</div><div><div></div><div>83%</div><div>16%</div><div>.</div></div></div>
2	D	140	<div><div>%</div><div><div></div><div>71%</div><div>27%</div><div>.</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

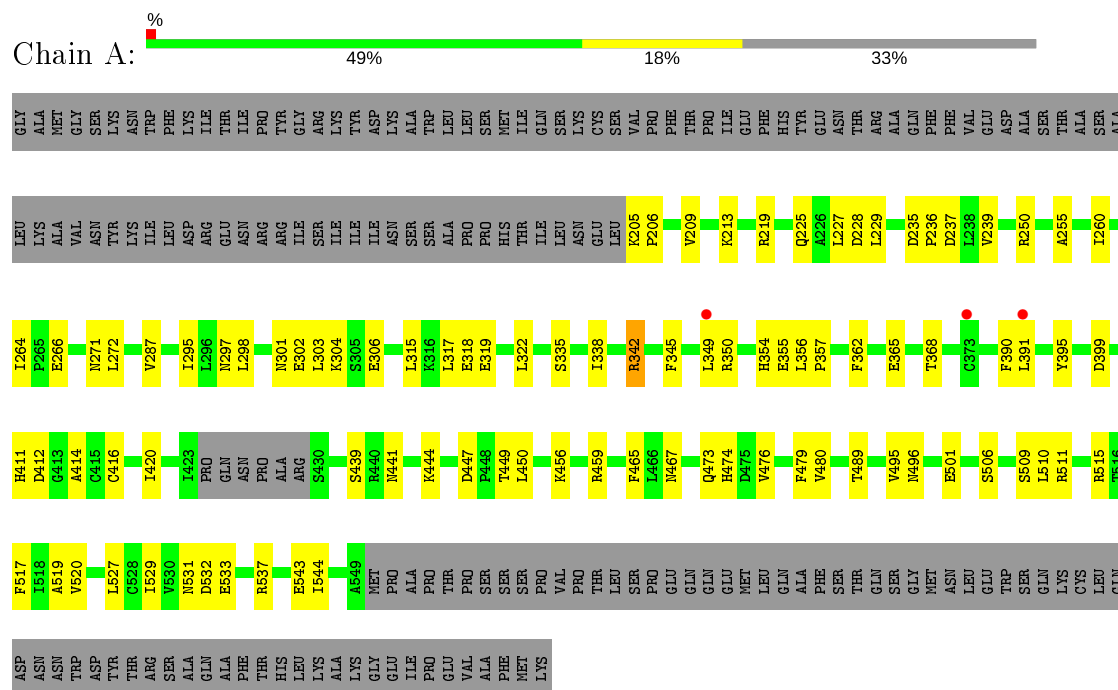
Continued from previous page...

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

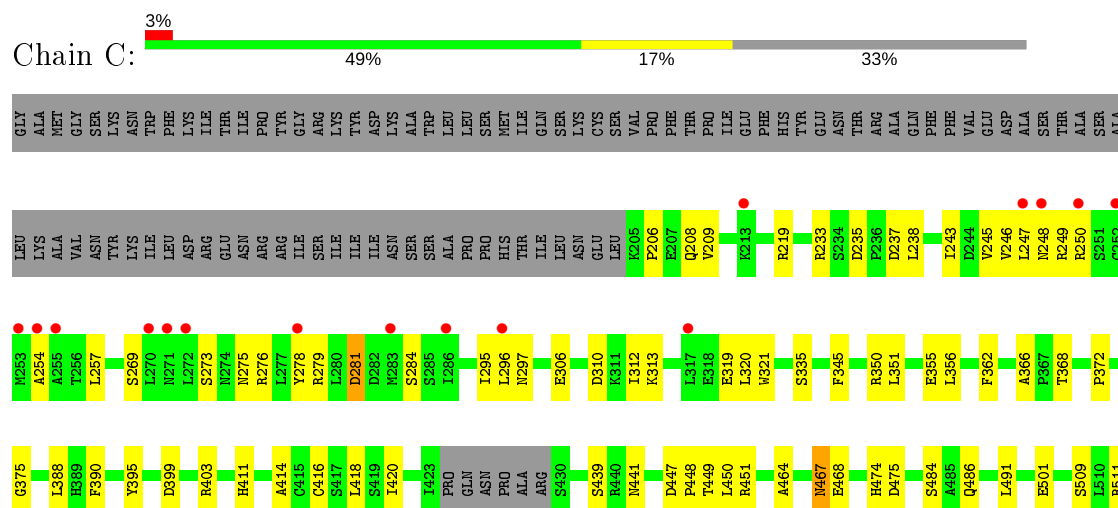
3 Residue-property plots

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.

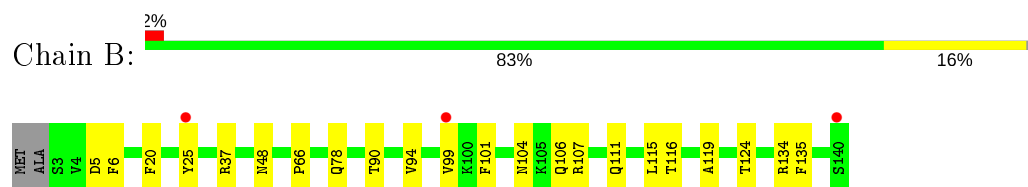
• Molecule 1: Nuclear RNA export factor 1



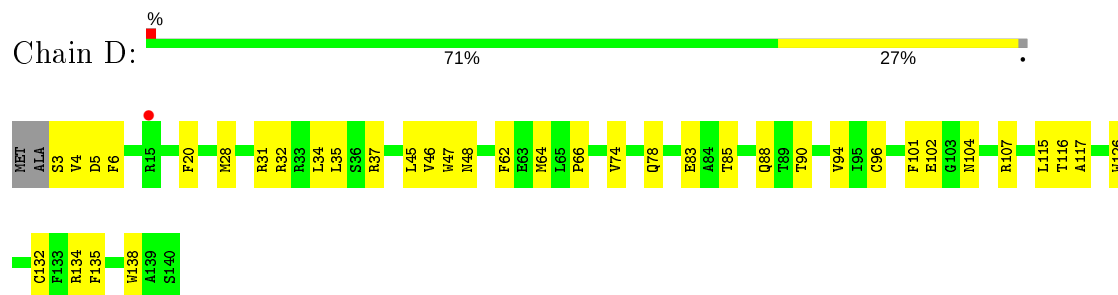
• Molecule 1: Nuclear RNA export factor 1



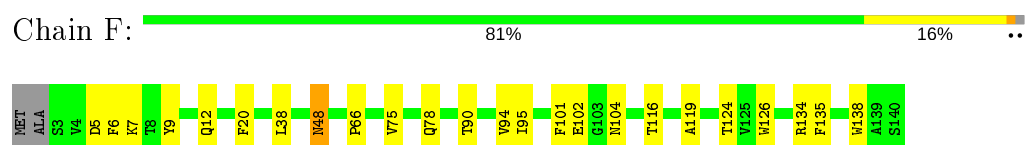
- Molecule 2: NTF2-related export protein 1



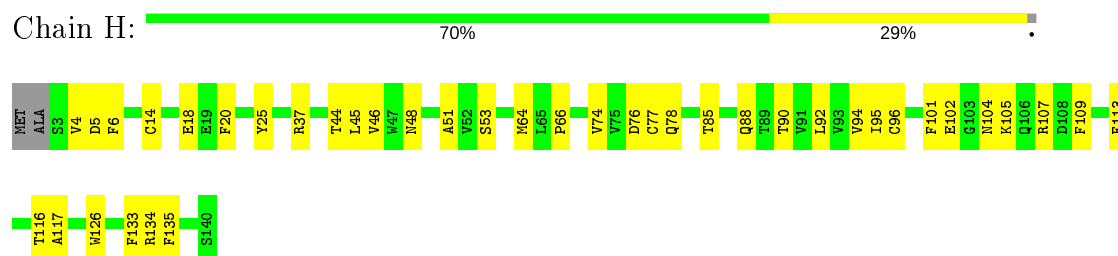
- Molecule 2: NTF2-related export protein 1



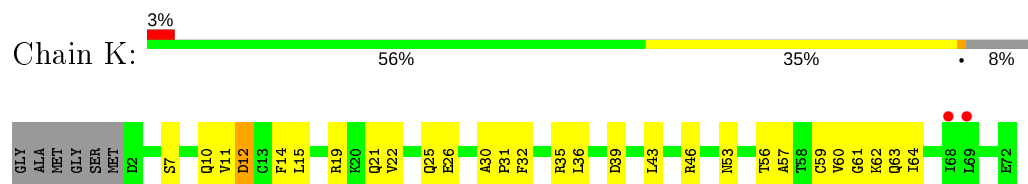
- Molecule 2: NTF2-related export protein 1



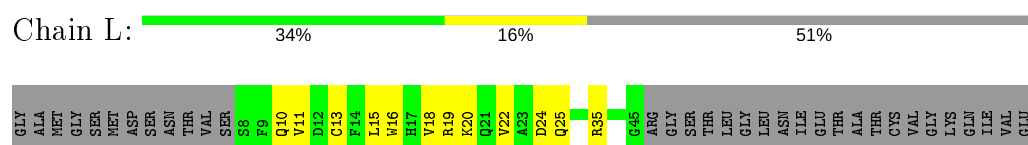
- Molecule 2: NTF2-related export protein 1



- Molecule 3: Non-structural protein 1

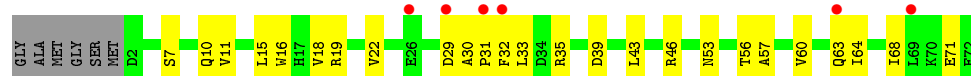


- Molecule 3: Non-structural protein 1

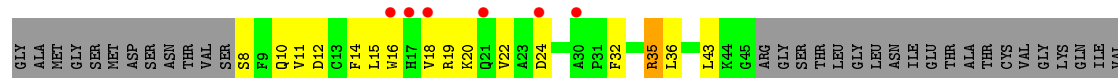
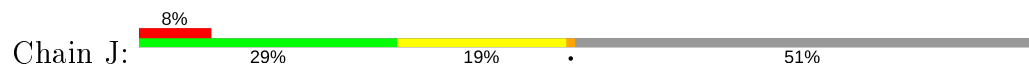


GLU

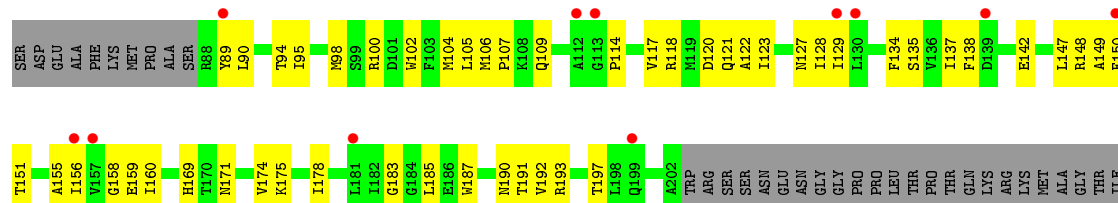
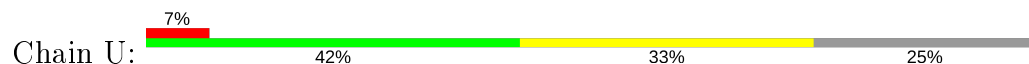
- Molecule 3: Non-structural protein 1



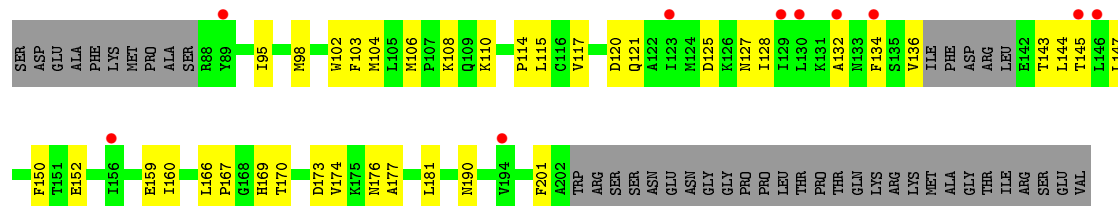
- Molecule 3: Non-structural protein 1

GLU
ARG
ILE
LEU
LYS
GLU
GLU

- Molecule 4: Non-structural protein 1

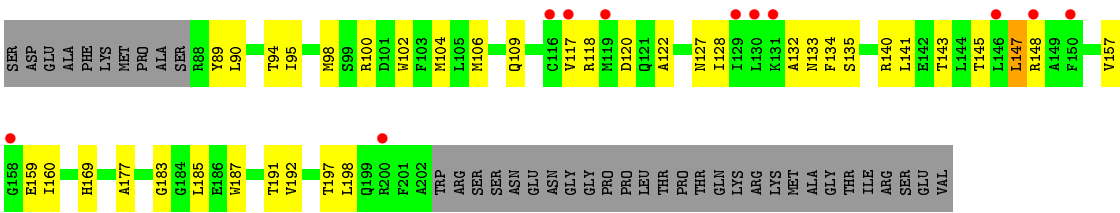
ARG
SER
GLU
VAL

- Molecule 4: Non-structural protein 1

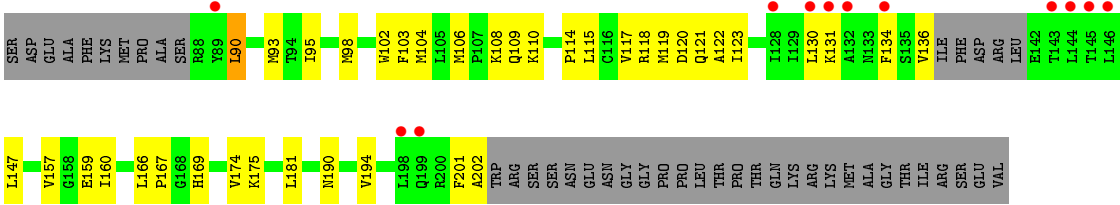


- Molecule 4: Non-structural protein 1





● 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.

All (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
3:L:15:LEU:HD22	3:M:15:LEU:HD22	1.68	0.75
1:G:211:GLN:HG3	1:G:241:GLN:HE22	1.50	0.75
4:X:132:ALA:HB2	4:X:147:LEU:HD23	1.69	0.74
1:E:537:ARG:NH2	1:E:543:GLU:OE2	2.18	0.74
3:K:63:GLN:HE22	4:X:197:THR:HG22	1.51	0.74
3:K:10:GLN:HA	3:K:57:ALA:HB1	1.69	0.73
3:M:10:GLN:HA	3:M:57:ALA:HB1	1.68	0.73
1:A:225:GLN:HE22	1:A:266:GLU:HG2	1.53	0.73
1:C:208:GLN:HB3	1:C:243:ILE:HG12	1.71	0.72
4:U:128:ILE:O	4:U:193:ARG:N	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:129:ILE:HG12	4:U:193:ARG:HD2	1.71	0.72
3:K:19:ARG:HB3	3:K:36:LEU:HD21	1.72	0.71
1:G:264:ILE:HD12	1:G:267:LEU:HD13	1.71	0.71
1:A:537:ARG:NH2	1:A:543:GLU:OE2	2.23	0.70
1:A:391:LEU:HD11	1:A:495:VAL:HG21	1.74	0.70
4:V:106:MET:HB2	4:V:121:GLN:H	1.57	0.70
4:X:132:ALA:HB3	4:X:198:LEU:HD21	1.74	0.69
1:A:219:ARG:NH1	1:A:237:ASP:OD2	2.25	0.69
1:E:287:VAL:HG22	1:E:315:LEU:HG	1.74	0.69
1:C:350:ARG:HG2	1:C:355:GLU:HA	1.75	0.68
2:H:90:THR:HG22	2:H:116:THR:HG22	1.74	0.68
4:X:140:ARG:NH1	4:X:141:LEU:O	2.27	0.67
1:C:509:SER:HB3	1:C:511:ARG:HH21	1.60	0.67
1:G:509:SER:HB3	1:G:511:ARG:HH21	1.59	0.67
2:H:102:GLU:O	2:H:104:ASN:ND2	2.28	0.67
4:U:95:ILE:HA	4:U:98:MET:HB2	1.76	0.67
1:A:350:ARG:HG2	1:A:355:GLU:HA	1.76	0.66
2:H:85:THR:HB	2:H:88:GLN:HB2	1.77	0.66
3:L:35:ARG:HH12	3:M:46:ARG:HH12	1.43	0.66
4:V:170:THR:OG1	4:V:173:ASP:OD2	2.13	0.66
3:J:35:ARG:HH12	3:J:36:LEU:HB2	1.60	0.66
1:A:287:VAL:HG22	1:A:315:LEU:HG	1.77	0.66
1:A:365:GLU:HG3	2:D:37:ARG:HB3	1.78	0.66
1:A:531:ASN:HD22	2:B:78:GLN:HE21	1.44	0.66
1:C:390:PHE:HZ	1:C:529:ILE:HD11	1.60	0.65
1:G:390:PHE:HZ	1:G:529:ILE:HD11	1.61	0.65
4:Y:115:LEU:HD21	4:Y:174:VAL:HG22	1.79	0.65
1:A:390:PHE:HZ	1:A:529:ILE:HD11	1.60	0.64
4:Y:136:VAL:HG21	4:Y:201:PHE:CD1	2.32	0.64
1:A:213:LYS:HE2	4:U:137:ILE:HG21	1.79	0.64
4:V:144:LEU:HD11	4:V:174:VAL:HG22	1.80	0.64
4:Y:123:ILE:O	4:Y:190:ASN:ND2	2.31	0.63
2:D:74:VAL:HG22	2:D:96:CYS:HB3	1.80	0.63
1:G:218:LYS:HE3	1:G:237:ASP:OD2	1.98	0.63
4:U:94:THR:O	4:U:98:MET:N	2.32	0.63
4:Y:109:GLN:HG2	4:Y:118:ARG:HG2	1.79	0.63
1:C:295:ILE:HG23	1:C:319:GLU:HB3	1.79	0.63
3:M:29:ASP:O	3:M:33:LEU:N	2.23	0.63
1:A:272:LEU:O	1:A:301:ASN:ND2	2.29	0.63
4:X:127:ASN:OD1	4:X:191:THR:OG1	2.15	0.63
1:E:533:GLU:HG2	2:F:94:VAL:HG21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:LEU:HB3	1:E:283:MET:HB2	1.79	0.62
1:G:284:SER:HA	1:G:312:ILE:HG22	1.80	0.62
4:U:106:MET:HB2	4:U:121:GLN:H	1.63	0.62
1:G:295:ILE:HG23	1:G:319:GLU:HB3	1.81	0.62
1:E:510:LEU:HD23	1:E:544:ILE:HG12	1.80	0.62
1:G:215:ILE:HA	1:G:218:LYS:HD3	1.81	0.62
4:V:143:THR:HA	4:V:169:HIS:HB3	1.81	0.62
3:M:11:VAL:O	3:M:15:LEU:HG	1.99	0.61
4:U:147:LEU:HD13	4:U:160:ILE:HD12	1.82	0.61
1:E:229:LEU:HA	1:E:232:LEU:HD13	1.83	0.61
3:K:35:ARG:NH1	3:J:12:ASP:OD2	2.34	0.61
2:B:90:THR:HG22	2:B:116:THR:HG22	1.83	0.61
1:C:254:ALA:HA	1:C:257:LEU:HD12	1.83	0.60
1:C:520:VAL:HG11	2:D:83:GLU:HG2	1.83	0.60
1:G:219:ARG:NH1	1:G:235:ASP:OD1	2.34	0.60
4:U:100:ARG:O	4:U:148:ARG:NH1	2.35	0.60
2:H:107:ARG:HD3	2:H:135:PHE:CE2	2.36	0.60
3:K:53:ASN:HB2	4:X:94:THR:HG21	1.83	0.60
4:Y:175:LYS:HG2	4:Y:202:ALA:HB1	1.82	0.60
1:C:249:ARG:HH22	1:G:372:PRO:HA	1.67	0.60
1:G:287:VAL:HG22	1:G:315:LEU:HG	1.82	0.60
2:D:102:GLU:O	2:D:104:ASN:ND2	2.34	0.60
4:Y:130:LEU:HD12	4:Y:194:VAL:HG22	1.83	0.60
3:J:19:ARG:HH11	3:J:35:ARG:NH2	2.00	0.59
1:C:233:ARG:HA	1:C:238:LEU:HD12	1.85	0.59
3:K:22:VAL:O	3:K:26:GLU:N	2.34	0.59
1:E:531:ASN:HD22	2:F:78:GLN:HE21	1.50	0.59
1:C:515:ARG:NH1	1:C:532:ASP:OD2	2.35	0.59
1:E:253:MET:HG2	1:E:283:MET:HG2	1.85	0.59
4:X:106:MET:N	4:X:120:ASP:OD1	2.31	0.59
1:C:219:ARG:NH1	1:C:235:ASP:OD2	2.35	0.59
3:M:19:ARG:NH2	3:M:39:ASP:OD2	2.35	0.59
3:M:43:LEU:HD23	3:M:46:ARG:HD2	1.83	0.59
4:U:102:TRP:HZ2	4:U:159:GLU:HB2	1.68	0.58
4:Y:90:LEU:HD11	4:Y:201:PHE:CE2	2.38	0.58
1:C:238:LEU:HD21	1:C:245:VAL:HG22	1.86	0.58
3:K:14:PHE:HB2	3:K:61:GLY:HA3	1.85	0.58
1:G:521:PRO:HD3	4:V:103:PHE:CE2	2.38	0.58
3:J:35:ARG:NH1	3:J:36:LEU:N	2.52	0.58
2:F:48:ASN:ND2	2:F:134:ARG:HA	2.18	0.58
4:Y:95:ILE:HA	4:Y:98:MET:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:VAL:HG13	1:C:521:PRO:HD2	1.85	0.58
1:C:416:CYS:HA	1:C:532:ASP:O	2.03	0.58
4:U:106:MET:HG2	4:U:122:ALA:HB2	1.86	0.58
4:X:109:GLN:HG2	4:X:118:ARG:HG2	1.86	0.58
1:A:338:ILE:O	1:A:342:ARG:HD3	2.04	0.57
1:E:271:ASN:OD1	1:E:297:ASN:ND2	2.30	0.57
1:E:399:ASP:OD2	1:E:473:GLN:HA	2.05	0.57
4:V:108:LYS:HE2	4:V:110:LYS:NZ	2.19	0.57
1:E:285:SER:O	1:E:289:LYS:NZ	2.31	0.57
1:E:209:VAL:HG13	1:E:259:ILE:HD11	1.87	0.57
1:G:447:ASP:OD1	1:G:449:THR:HG22	2.05	0.57
3:L:11:VAL:HG11	3:M:32:PHE:HE1	1.69	0.57
3:J:35:ARG:NH1	3:J:36:LEU:HB2	2.20	0.57
1:A:315:LEU:HD13	1:A:317:LEU:HD21	1.85	0.57
1:A:533:GLU:HG2	2:B:94:VAL:HG21	1.86	0.57
2:H:107:ARG:HD3	2:H:135:PHE:CD2	2.39	0.57
3:J:35:ARG:HH11	3:J:36:LEU:N	2.02	0.57
1:G:313:LYS:HA	1:G:345:PHE:CE2	2.40	0.56
4:V:108:LYS:HD2	4:V:121:GLN:HG3	1.87	0.56
4:X:183:GLY:O	4:X:187:TRP:HD1	1.88	0.56
4:X:106:MET:HG2	4:X:122:ALA:HB2	1.87	0.56
1:C:208:GLN:HB3	1:C:243:ILE:CG1	2.34	0.56
2:D:90:THR:HG22	2:D:116:THR:HG22	1.86	0.56
3:K:56:THR:HG23	4:X:94:THR:HG23	1.88	0.56
4:U:127:ASN:OD1	4:U:191:THR:OG1	2.17	0.56
4:X:89:TYR:CE2	4:X:135:SER:HB3	2.40	0.56
4:X:117:VAL:HG22	4:X:160:ILE:HG12	1.88	0.56
1:A:271:ASN:OD1	1:A:297:ASN:ND2	2.33	0.56
3:M:29:ASP:CB	3:M:32:PHE:HB3	2.27	0.56
4:Y:106:MET:HB2	4:Y:121:GLN:H	1.70	0.56
1:A:235:ASP:O	1:A:237:ASP:N	2.35	0.56
4:X:133:ASN:O	4:X:145:THR:OG1	2.20	0.56
1:G:533:GLU:HG2	2:H:94:VAL:HG21	1.87	0.55
3:K:21:GLN:O	3:K:25:GLN:NE2	2.40	0.55
4:V:134:PHE:HE1	4:V:145:THR:H	1.55	0.55
1:A:315:LEU:HB2	1:A:345:PHE:HZ	1.72	0.55
1:C:208:GLN:OE1	1:C:243:ILE:HD13	2.06	0.55
2:D:31:ARG:HB3	2:D:34:LEU:HD12	1.88	0.55
3:M:15:LEU:O	3:M:19:ARG:HG3	2.07	0.55
2:D:85:THR:HB	2:D:88:GLN:HB2	1.89	0.55
1:E:412:ASP:HA	1:E:459:ARG:HD2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:25:TYR:HE2	2:H:95:ILE:HD13	1.71	0.55
1:G:350:ARG:HG2	1:G:355:GLU:HA	1.88	0.55
4:U:185:LEU:HB3	4:U:192:VAL:HG21	1.89	0.55
4:X:128:ILE:HD13	4:X:157:VAL:HG11	1.89	0.55
1:A:412:ASP:HA	1:A:459:ARG:HD2	1.89	0.55
1:G:531:ASN:HD22	2:H:78:GLN:HE21	1.54	0.55
4:X:100:ARG:O	4:X:148:ARG:NH1	2.40	0.54
4:U:171:ASN:ND2	4:U:175:LYS:HE3	2.22	0.54
1:A:315:LEU:HB2	1:A:345:PHE:CZ	2.42	0.54
1:C:313:LYS:HA	1:C:345:PHE:CE2	2.43	0.54
1:E:390:PHE:HZ	1:E:529:ILE:HD11	1.72	0.54
4:Y:108:LYS:HB3	4:Y:110:LYS:NZ	2.23	0.54
1:C:273:SER:HB3	1:C:297:ASN:ND2	2.22	0.54
1:C:447:ASP:OD1	1:C:449:THR:HG22	2.07	0.54
1:G:448:PRO:HA	1:G:451:ARG:HD2	1.90	0.54
3:M:30:ALA:HB3	3:M:31:PRO:HD3	1.88	0.54
2:D:117:ALA:HB2	2:D:126:TRP:CE2	2.42	0.54
1:C:269:SER:HB2	1:C:295:ILE:HD12	1.89	0.54
1:C:531:ASN:HD22	2:D:78:GLN:HB3	1.73	0.54
2:D:66:PRO:HB2	2:D:101:PHE:HD2	1.72	0.53
1:G:238:LEU:HD11	1:G:244:ASP:HA	1.90	0.53
4:V:160:ILE:CD1	4:V:177:ALA:HB1	2.38	0.53
1:G:297:ASN:HD22	1:G:298:LEU:N	2.06	0.53
1:G:416:CYS:HA	1:G:532:ASP:O	2.09	0.53
3:M:63:GLN:HE22	4:U:197:THR:HA	1.73	0.53
1:G:228:ASP:HA	1:G:271:ASN:HB3	1.89	0.53
4:U:171:ASN:HD21	4:U:175:LYS:HE3	1.73	0.53
2:B:119:ALA:HA	2:B:124:THR:HG22	1.89	0.53
2:B:48:ASN:ND2	2:B:134:ARG:HA	2.24	0.53
2:D:107:ARG:HD3	2:D:135:PHE:CE2	2.43	0.53
4:V:115:LEU:HD12	4:V:173:ASP:HB3	1.90	0.53
4:V:95:ILE:HA	4:V:98:MET:HB2	1.91	0.53
2:B:66:PRO:HB2	2:B:101:PHE:HD2	1.73	0.52
2:F:66:PRO:HB2	2:F:101:PHE:HD2	1.74	0.52
1:G:238:LEU:HD11	1:G:245:VAL:H	1.74	0.52
1:G:418:LEU:HD12	1:G:534:LEU:O	2.09	0.52
4:U:104:MET:HB3	4:U:107:PRO:HG3	1.91	0.52
2:H:66:PRO:HB3	2:H:102:GLU:HB3	1.90	0.52
4:Y:119:MET:HG2	4:Y:181:LEU:HD22	1.90	0.52
1:C:519:ALA:HB1	1:C:527:LEU:HB2	1.91	0.52
3:M:19:ARG:HG2	3:M:32:PHE:CZ	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:HD12	1:C:534:LEU:O	2.09	0.52
4:X:102:TRP:CZ3	4:X:104:MET:HE2	2.45	0.52
1:A:225:GLN:NE2	1:A:266:GLU:HG2	2.23	0.52
3:K:53:ASN:O	3:K:56:THR:OG1	2.26	0.52
4:V:117:VAL:HG13	4:V:181:LEU:HD21	1.90	0.52
1:E:362:PHE:CZ	2:H:20:PHE:HB2	2.45	0.52
4:V:114:PRO:HA	4:V:166:LEU:HD13	1.91	0.52
1:C:540:SER:HB2	1:C:543:GLU:HG3	1.91	0.52
2:D:47:TRP:CE3	2:D:48:ASN:HB2	2.44	0.52
3:K:59:CYS:HA	3:K:62:LYS:HG3	1.92	0.52
1:C:395:TYR:CE2	1:C:474:HIS:CE1	2.97	0.51
3:M:16:TRP:HA	3:M:19:ARG:HD2	1.92	0.51
4:U:90:LEU:HD12	4:U:134:PHE:CE1	2.45	0.51
2:H:74:VAL:HG22	2:H:96:CYS:HB3	1.91	0.51
1:C:531:ASN:HD22	2:D:78:GLN:HE21	1.57	0.51
4:V:144:LEU:H	4:V:169:HIS:CD2	2.28	0.51
1:E:246:VAL:HG12	1:E:248:ASN:H	1.75	0.51
1:G:395:TYR:CE2	1:G:474:HIS:CE1	2.97	0.51
1:A:399:ASP:OD2	1:A:473:GLN:HA	2.10	0.51
1:A:411:HIS:O	1:A:459:ARG:HB3	2.10	0.51
1:E:257:LEU:HB3	1:E:289:LYS:HD3	1.92	0.51
4:V:173:ASP:HA	4:V:176:ASN:OD1	2.10	0.51
2:B:90:THR:HA	2:B:115:LEU:O	2.11	0.51
4:U:118:ARG:O	4:U:158:GLY:HA2	2.11	0.51
3:K:14:PHE:CE1	3:K:62:LYS:HG2	2.46	0.51
4:V:128:ILE:HA	4:V:150:PHE:O	2.11	0.51
1:C:486:GLN:HG3	1:C:491:LEU:HD13	1.93	0.50
1:G:218:LYS:HB3	1:G:218:LYS:NZ	2.27	0.50
1:A:298:LEU:HB2	1:A:322:LEU:HD23	1.93	0.50
1:C:368:THR:OG1	2:D:102:GLU:O	2.28	0.50
1:E:280:LEU:HD22	1:E:283:MET:SD	2.51	0.50
3:J:35:ARG:HH12	3:J:36:LEU:CB	2.25	0.50
1:G:488:SER:HA	4:V:103:PHE:HB2	1.93	0.50
2:F:119:ALA:HA	2:F:124:THR:HG22	1.92	0.50
1:G:306:GLU:OE2	1:G:306:GLU:N	2.30	0.50
1:C:448:PRO:HA	1:C:451:ARG:HD2	1.92	0.50
1:C:515:ARG:HD2	1:C:532:ASP:OD1	2.11	0.50
1:E:233:ARG:NH1	1:E:276:ARG:HG3	2.27	0.50
2:H:95:ILE:HD12	2:H:113:PHE:HE2	1.76	0.50
3:J:19:ARG:HH11	3:J:35:ARG:HH21	1.59	0.50
4:X:90:LEU:HD12	4:X:134:PHE:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:94:THR:O	4:X:98:MET:N	2.45	0.50
4:Y:123:ILE:HD12	4:Y:157:VAL:HG13	1.94	0.49
1:C:235:ASP:O	1:C:237:ASP:N	2.45	0.49
3:L:15:LEU:O	3:L:19:ARG:HG3	2.12	0.49
1:A:447:ASP:OD1	1:A:449:THR:HG22	2.12	0.49
1:G:531:ASN:HD22	2:H:78:GLN:HB3	1.77	0.49
1:A:227:LEU:HD22	1:A:260:ILE:HD11	1.94	0.49
1:C:475:ASP:HB2	1:C:548:PHE:CE1	2.47	0.49
1:E:279:ARG:HB2	1:E:281:ASP:OD1	2.12	0.49
3:L:35:ARG:HH12	3:M:46:ARG:NH1	2.09	0.49
4:V:110:LYS:HB2	4:V:117:VAL:HB	1.94	0.49
1:E:531:ASN:HD22	2:F:78:GLN:HB3	1.78	0.49
3:L:25:GLN:NE2	3:M:71:GLU:OE1	2.45	0.49
4:V:147:LEU:O	4:V:159:GLU:HA	2.12	0.49
4:Y:175:LYS:HE2	4:Y:202:ALA:HA	1.93	0.49
1:G:519:ALA:HB1	1:G:527:LEU:HB2	1.94	0.49
4:U:137:ILE:HG22	4:U:138:PHE:CD2	2.48	0.49
4:Y:102:TRP:HZ3	4:Y:104:MET:HG2	1.77	0.49
1:C:276:ARG:NH1	1:C:278:TYR:OH	2.45	0.49
1:E:366:ALA:HB1	2:F:102:GLU:OE2	2.13	0.49
1:G:208:GLN:HG2	1:G:243:ILE:HG21	1.95	0.49
1:G:432:LEU:HD21	1:G:538:ASN:HB3	1.95	0.49
1:G:440:ARG:HB3	2:H:76:ASP:OD2	2.12	0.49
1:A:510:LEU:HD23	1:A:544:ILE:HG12	1.95	0.49
1:C:320:LEU:O	1:C:351:LEU:HA	2.13	0.49
1:E:447:ASP:OD1	1:E:449:THR:HG22	2.13	0.49
2:H:25:TYR:CE2	2:H:95:ILE:HD13	2.48	0.49
4:V:114:PRO:HD2	4:V:173:ASP:OD2	2.12	0.49
1:A:531:ASN:HD22	2:B:78:GLN:HB3	1.78	0.48
4:U:117:VAL:HG22	4:U:160:ILE:HG12	1.94	0.48
3:K:30:ALA:HB3	3:K:31:PRO:HD3	1.94	0.48
1:A:480:VAL:HB	1:A:496:ASN:HB2	1.96	0.48
4:Y:106:MET:N	4:Y:120:ASP:OD1	2.44	0.48
2:B:5:ASP:OD1	2:B:6:PHE:N	2.47	0.48
1:G:416:CYS:O	1:G:455:LEU:HD12	2.14	0.48
4:U:114:PRO:HG2	4:U:169:HIS:HB3	1.94	0.48
1:A:355:GLU:HB3	2:D:4:VAL:HG22	1.95	0.48
1:G:399:ASP:OD1	1:G:474:HIS:HD2	1.96	0.48
1:G:475:ASP:HB2	1:G:548:PHE:CE1	2.48	0.48
4:Y:117:VAL:CG1	4:Y:181:LEU:HD21	2.44	0.48
1:E:515:ARG:HG2	1:E:517:PHE:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:MET:O	2:D:64:MET:HG2	2.12	0.48
1:E:219:ARG:NH1	1:E:235:ASP:OD2	2.46	0.48
1:G:214:LEU:O	1:G:218:LYS:HG3	2.13	0.48
4:V:115:LEU:HD21	4:V:160:ILE:HD13	1.94	0.48
1:A:489:THR:O	1:A:520:VAL:HG23	2.13	0.48
1:E:415:CYS:HB3	1:E:455:LEU:HD11	1.95	0.48
1:G:476:VAL:HG13	1:G:479:PHE:CD2	2.49	0.48
3:K:60:VAL:HG12	3:K:64:ILE:HD11	1.96	0.48
1:C:532:ASP:H	2:D:78:GLN:HE22	1.60	0.48
1:C:533:GLU:HG2	2:D:94:VAL:HG21	1.95	0.48
4:V:108:LYS:HE2	4:V:110:LYS:HZ3	1.78	0.48
1:A:411:HIS:HB3	1:A:414:ALA:HB2	1.96	0.47
4:X:160:ILE:HD13	4:X:177:ALA:HB1	1.95	0.47
3:L:11:VAL:HG11	3:M:32:PHE:CE1	2.49	0.47
4:Y:114:PRO:HG2	4:Y:169:HIS:HA	1.95	0.47
1:C:411:HIS:H	1:C:414:ALA:HB2	1.78	0.47
1:A:362:PHE:CZ	2:D:20:PHE:HB2	2.48	0.47
1:G:297:ASN:ND2	1:G:321:TRP:HB2	2.29	0.47
1:G:327:LEU:O	1:G:330:THR:HG22	2.14	0.47
3:J:32:PHE:CE2	3:J:35:ARG:NH2	2.82	0.47
3:K:12:ASP:O	3:K:15:LEU:HG	2.14	0.47
4:Y:90:LEU:HB2	4:Y:134:PHE:H	1.80	0.47
4:Y:160:ILE:HG13	4:Y:181:LEU:HD11	1.97	0.47
1:G:540:SER:HB2	1:G:543:GLU:HG3	1.96	0.47
1:E:414:ALA:HA	1:E:530:VAL:O	2.15	0.47
2:F:90:THR:HG22	2:F:116:THR:HA	1.96	0.47
1:G:440:ARG:NH1	2:H:77:CYS:O	2.47	0.47
1:C:296:LEU:O	1:C:320:LEU:HA	2.15	0.47
1:G:297:ASN:ND2	1:G:299:SER:H	2.13	0.47
4:X:143:THR:HA	4:X:169:HIS:NE2	2.29	0.47
1:A:476:VAL:HG13	1:A:479:PHE:CD2	2.50	0.47
4:U:183:GLY:O	4:U:187:TRP:HD1	1.97	0.47
4:Y:147:LEU:O	4:Y:159:GLU:HG2	2.14	0.47
1:A:209:VAL:HG22	1:A:255:ALA:HB1	1.97	0.47
1:C:279:ARG:HB2	1:C:281:ASP:OD1	2.14	0.47
1:E:391:LEU:HD11	1:E:495:VAL:HG21	1.97	0.47
1:G:279:ARG:HB2	1:G:281:ASP:OD1	2.15	0.47
1:E:515:ARG:HD2	1:E:532:ASP:OD1	2.15	0.47
1:A:264:ILE:HG22	1:A:266:GLU:OE2	2.15	0.47
1:A:509:SER:HB3	1:A:511:ARG:HH21	1.79	0.47
1:A:515:ARG:HG2	1:A:517:PHE:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:174:VAL:O	4:U:178:ILE:HG12	2.15	0.47
1:C:464:ALA:O	1:C:468:GLU:HG2	2.16	0.46
1:A:447:ASP:HB3	1:A:450:LEU:HB2	1.96	0.46
1:E:476:VAL:HG13	1:E:479:PHE:CD2	2.51	0.46
1:G:218:LYS:NZ	1:G:218:LYS:CB	2.78	0.46
1:C:521:PRO:HD3	4:Y:103:PHE:CE2	2.50	0.46
1:G:218:LYS:HB3	1:G:218:LYS:HZ3	1.78	0.46
1:G:313:LYS:HA	1:G:345:PHE:HE2	1.80	0.46
1:G:403:ARG:N	1:G:467:ASN:HD21	2.13	0.46
3:M:60:VAL:HG12	3:M:64:ILE:HD11	1.97	0.46
4:X:95:ILE:HA	4:X:98:MET:HB2	1.97	0.46
4:U:128:ILE:HG23	4:U:149:ALA:HB1	1.97	0.46
4:X:135:SER:OG	4:X:143:THR:OG1	2.26	0.46
1:C:297:ASN:OD1	1:C:321:TRP:HB2	2.16	0.46
2:F:20:PHE:HB2	1:G:362:PHE:CZ	2.51	0.46
1:C:247:LEU:HD12	1:C:275:ASN:HB3	1.97	0.46
1:E:333:ASP:N	1:E:333:ASP:OD1	2.49	0.46
4:X:106:MET:CG	4:X:122:ALA:HB2	2.46	0.46
2:H:64:MET:O	2:H:64:MET:HG2	2.15	0.46
3:J:43:LEU:HD23	3:J:43:LEU:HA	1.80	0.46
1:C:441:ASN:ND2	2:D:74:VAL:HG12	2.30	0.46
2:H:48:ASN:ND2	2:H:134:ARG:HA	2.31	0.46
2:H:14:CYS:O	2:H:18:GLU:HG2	2.16	0.46
1:C:351:LEU:HB3	1:C:356:LEU:HD21	1.97	0.46
1:C:403:ARG:N	1:C:467:ASN:HD21	2.14	0.46
1:C:501:GLU:OE2	1:C:511:ARG:NH1	2.49	0.46
2:H:109:PHE:CD2	2:H:133:PHE:HE1	2.33	0.46
4:X:128:ILE:O	4:X:192:VAL:HA	2.16	0.46
3:M:53:ASN:O	3:M:56:THR:OG1	2.35	0.45
1:G:520:VAL:CG1	1:G:521:PRO:HD2	2.46	0.45
1:A:318:GLU:O	1:A:349:LEU:N	2.37	0.45
1:E:356:LEU:HD23	1:E:357:PRO:HD2	1.98	0.45
1:G:297:ASN:C	1:G:297:ASN:HD22	2.19	0.45
1:G:532:ASP:H	2:H:78:GLN:HE22	1.63	0.45
1:A:416:CYS:HA	1:A:532:ASP:O	2.16	0.45
2:D:5:ASP:OD1	2:D:6:PHE:N	2.49	0.45
1:G:414:ALA:HA	1:G:530:VAL:O	2.16	0.45
3:M:56:THR:HG23	4:U:94:THR:HG23	1.97	0.45
2:D:74:VAL:CG2	2:D:96:CYS:HB3	2.47	0.45
2:H:37:ARG:HD3	2:H:37:ARG:HA	1.79	0.45
4:V:125:ASP:N	4:V:190:ASN:OD1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:THR:O	2:B:104:ASN:ND2	2.31	0.45
1:G:320:LEU:O	1:G:351:LEU:HA	2.16	0.45
1:G:515:ARG:HG2	1:G:517:PHE:CE2	2.52	0.45
3:K:43:LEU:HD23	3:K:46:ARG:HD2	1.98	0.45
1:G:208:GLN:HG2	1:G:243:ILE:CG2	2.47	0.45
1:C:420:ILE:HG12	1:C:439:SER:HB2	1.98	0.45
1:G:220:TYR:HE1	1:G:267:LEU:HD11	1.81	0.45
2:D:20:PHE:CD1	2:D:115:LEU:HD21	2.51	0.45
2:H:90:THR:HG22	2:H:116:THR:CG2	2.46	0.45
1:C:515:ARG:HG2	1:C:517:PHE:CZ	2.51	0.45
4:U:89:TYR:CE1	4:U:135:SER:HB3	2.52	0.45
1:A:420:ILE:HG12	1:A:439:SER:HB2	1.99	0.44
1:C:375:GLY:HA2	2:D:138:TRP:CH2	2.53	0.44
2:D:107:ARG:HD3	2:D:135:PHE:CD2	2.51	0.44
2:H:44:THR:HG22	2:H:53:SER:OG	2.16	0.44
3:J:18:VAL:O	3:J:22:VAL:HG23	2.18	0.44
4:U:109:GLN:HG2	4:U:118:ARG:HG2	1.98	0.44
4:V:106:MET:N	4:V:120:ASP:OD1	2.48	0.44
2:B:20:PHE:HB2	1:C:362:PHE:CZ	2.52	0.44
3:J:8:SER:N	3:J:11:VAL:HG12	2.32	0.44
3:K:60:VAL:O	3:K:64:ILE:HG13	2.17	0.44
4:V:132:ALA:HB2	4:V:147:LEU:HD23	1.98	0.44
4:V:114:PRO:HG3	4:V:167:PRO:HD2	1.98	0.44
1:A:298:LEU:HB3	1:A:303:LEU:HD11	1.98	0.44
2:F:48:ASN:HD21	2:F:134:ARG:HA	1.79	0.44
2:F:135:PHE:HB2	2:F:138:TRP:HB3	1.98	0.44
2:F:5:ASP:OD1	2:F:6:PHE:N	2.50	0.44
3:K:15:LEU:O	3:K:19:ARG:HG3	2.17	0.44
3:L:25:GLN:NE2	3:M:68:ILE:HG23	2.32	0.44
3:M:18:VAL:O	3:M:22:VAL:HG23	2.17	0.44
1:G:395:TYR:HE2	1:G:474:HIS:CE1	2.35	0.44
4:U:127:ASN:O	4:U:151:THR:HA	2.17	0.44
4:X:102:TRP:HZ3	4:X:104:MET:HE2	1.82	0.44
2:B:25:TYR:OH	2:B:111:GLN:OE1	2.24	0.44
2:F:126:TRP:HD1	1:G:361:ALA:H	1.66	0.44
3:J:15:LEU:O	3:J:19:ARG:HG3	2.17	0.44
1:G:388:LEU:HD23	1:G:388:LEU:HA	1.83	0.44
1:G:415:CYS:HB3	1:G:455:LEU:HD11	2.00	0.44
1:C:388:LEU:HD23	1:C:388:LEU:HA	1.75	0.44
1:C:306:GLU:OE2	1:C:306:GLU:N	2.33	0.43
1:C:515:ARG:HG2	1:C:517:PHE:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:GLU:OE2	1:E:306:GLU:N	2.40	0.43
1:C:447:ASP:HB3	1:C:450:LEU:HB2	2.00	0.43
2:F:102:GLU:O	2:F:104:ASN:ND2	2.51	0.43
4:Y:106:MET:HG2	4:Y:122:ALA:HB2	2.00	0.43
4:Y:108:LYS:O	4:Y:118:ARG:HA	2.18	0.43
1:A:395:TYR:CE1	1:A:474:HIS:CE1	3.06	0.43
2:B:90:THR:CG2	2:B:116:THR:HG22	2.46	0.43
1:C:246:VAL:HG22	1:C:248:ASN:H	1.82	0.43
4:U:129:ILE:O	4:U:149:ALA:HA	2.18	0.43
4:V:127:ASN:HB2	4:V:152:GLU:HG2	2.01	0.43
4:V:136:VAL:HG21	4:V:201:PHE:CD1	2.54	0.43
3:K:63:GLN:NE2	4:X:197:THR:HG22	2.26	0.43
1:C:206:PRO:HA	1:C:209:VAL:HB	2.01	0.43
1:C:399:ASP:OD1	1:C:474:HIS:HD2	2.01	0.43
3:J:19:ARG:HD3	3:J:35:ARG:NH2	2.34	0.43
3:J:35:ARG:HH11	3:J:36:LEU:H	1.65	0.43
3:M:7:SER:O	3:M:11:VAL:HG23	2.18	0.43
4:V:136:VAL:HG21	4:V:201:PHE:HB3	2.01	0.43
4:X:102:TRP:CZ2	4:X:159:GLU:HB2	2.53	0.43
1:E:315:LEU:HD13	1:E:317:LEU:HD21	1.99	0.43
2:F:38:LEU:HA	2:F:38:LEU:HD23	1.84	0.43
1:C:249:ARG:HH12	1:G:372:PRO:HA	1.82	0.43
2:F:90:THR:HG22	2:F:116:THR:HG22	2.00	0.43
3:K:19:ARG:NH1	3:K:39:ASP:OD2	2.51	0.43
4:U:129:ILE:HA	4:U:193:ARG:HB2	2.01	0.43
4:Y:108:LYS:HB3	4:Y:110:LYS:HZ2	1.83	0.43
2:H:45:LEU:HD12	2:H:46:VAL:N	2.34	0.43
3:K:7:SER:O	3:K:11:VAL:HG23	2.18	0.43
3:L:18:VAL:O	3:L:22:VAL:HG23	2.19	0.43
4:Y:102:TRP:CZ3	4:Y:104:MET:HG2	2.53	0.43
1:E:431:SER:O	1:E:511:ARG:NH2	2.51	0.43
1:G:486:GLN:HG3	1:G:491:LEU:HD13	2.01	0.42
4:U:150:PHE:HA	4:U:155:ALA:O	2.19	0.42
1:C:249:ARG:NH2	1:G:371:PRO:O	2.52	0.42
3:J:16:TRP:CZ3	3:J:20:LYS:HD2	2.54	0.42
3:K:19:ARG:HB3	3:K:36:LEU:CD2	2.47	0.42
4:U:128:ILE:N	4:U:191:THR:O	2.52	0.42
1:C:366:ALA:HB1	2:D:102:GLU:OE2	2.19	0.42
1:G:403:ARG:H	1:G:467:ASN:HD21	1.66	0.42
2:F:7:LYS:NZ	1:G:333:ASP:HB2	2.35	0.42
1:C:278:TYR:HE1	2:H:105:LYS:HD3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ASN:ND2	2:D:134:ARG:HA	2.34	0.42
4:V:108:LYS:HD2	4:V:121:GLN:CG	2.49	0.42
2:B:99:VAL:O	2:B:106:GLN:HG3	2.19	0.42
1:A:456:LYS:HG3	1:A:465:PHE:CD2	2.54	0.42
1:A:519:ALA:HB1	1:A:527:LEU:HB2	2.02	0.42
1:E:205:LYS:HA	1:E:206:PRO:HD3	1.91	0.42
1:E:355:GLU:HB3	2:H:4:VAL:HG22	2.01	0.42
1:E:432:LEU:HD23	1:E:511:ARG:NH1	2.34	0.42
1:C:372:PRO:HA	1:G:249:ARG:HH22	1.83	0.42
3:J:32:PHE:HE2	3:J:35:ARG:HH21	1.67	0.42
4:U:149:ALA:O	4:U:156:ILE:HA	2.19	0.42
1:C:484:SER:OG	2:D:132:CYS:HB2	2.20	0.42
1:A:354:HIS:HA	2:D:3:SER:O	2.19	0.42
4:U:128:ILE:HA	4:U:150:PHE:O	2.20	0.42
1:C:284:SER:HA	1:C:312:ILE:HG22	2.02	0.42
1:A:228:ASP:O	1:A:229:LEU:HD23	2.20	0.41
1:C:310:ASP:HA	1:C:313:LYS:HD3	2.01	0.41
2:D:28:MET:HG3	2:D:32:ARG:HE	1.85	0.41
1:E:321:TRP:CE3	1:E:352:ASP:HA	2.55	0.41
1:E:368:THR:OG1	2:F:102:GLU:O	2.15	0.41
2:H:5:ASP:OD1	2:H:6:PHE:N	2.53	0.41
2:D:35:LEU:HD23	2:D:62:PHE:CZ	2.55	0.41
1:G:515:ARG:NH1	1:G:532:ASP:OD2	2.53	0.41
1:A:441:ASN:ND2	1:A:444:LYS:HG2	2.34	0.41
2:B:37:ARG:HA	2:B:37:ARG:HD3	1.83	0.41
1:E:515:ARG:HG2	1:E:517:PHE:CZ	2.56	0.41
1:E:531:ASN:ND2	2:F:78:GLN:HE21	2.17	0.41
1:G:296:LEU:O	1:G:320:LEU:HA	2.19	0.41
3:K:32:PHE:O	3:K:36:LEU:HD23	2.20	0.41
3:M:19:ARG:HA	3:M:32:PHE:CZ	2.56	0.41
1:E:447:ASP:HB3	1:E:450:LEU:HD12	2.02	0.41
4:X:128:ILE:HG21	4:X:185:LEU:HD13	2.02	0.41
1:A:236:PRO:HB3	1:A:239:VAL:HB	2.03	0.41
1:A:501:GLU:OE1	1:A:506:SER:OG	2.39	0.41
4:V:102:TRP:HZ3	4:V:104:MET:HG2	1.85	0.41
2:D:45:LEU:HD12	2:D:46:VAL:N	2.35	0.41
1:E:284:SER:HA	1:E:312:ILE:HG22	2.02	0.41
1:G:403:ARG:HB2	1:G:467:ASN:ND2	2.36	0.41
4:U:105:LEU:N	4:U:120:ASP:OD1	2.53	0.41
1:A:515:ARG:HG2	1:A:517:PHE:CZ	2.56	0.41
2:F:12:GLN:HG3	1:G:357:PRO:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:LEU:O	2:H:51:ALA:HA	2.21	0.41
3:M:19:ARG:NH2	3:M:35:ARG:HB3	2.36	0.41
4:Y:166:LEU:HB3	4:Y:167:PRO:HD2	2.02	0.41
1:A:302:GLU:HB3	1:A:304:LYS:NZ	2.35	0.41
2:B:107:ARG:HD3	2:B:135:PHE:CD2	2.56	0.41
1:E:340:ALA:O	1:E:343:GLU:HB2	2.21	0.41
1:E:445:LEU:HD12	1:E:445:LEU:HA	1.86	0.41
2:H:117:ALA:HB2	2:H:126:TRP:CE2	2.56	0.41
1:E:362:PHE:CE1	2:H:126:TRP:HB2	2.56	0.41
4:U:89:TYR:CD1	4:U:135:SER:HB3	2.56	0.41
2:H:66:PRO:HB2	2:H:101:PHE:HD2	1.86	0.40
4:U:137:ILE:HG13	4:U:142:GLU:HB2	2.01	0.40
4:Y:147:LEU:O	4:Y:159:GLU:HA	2.21	0.40
1:A:228:ASP:HA	1:A:271:ASN:HB3	2.03	0.40
1:E:338:ILE:HG23	1:E:356:LEU:HD11	2.03	0.40
4:X:147:LEU:CD1	4:X:160:ILE:HD12	2.51	0.40
1:A:205:LYS:HA	1:A:206:PRO:HD3	1.90	0.40
1:C:520:VAL:CG1	1:C:521:PRO:HD2	2.51	0.40
1:E:420:ILE:HG12	1:E:439:SER:HB2	2.03	0.40
1:E:475:ASP:HB2	1:E:548:PHE:CE1	2.56	0.40
2:F:75:VAL:HG13	2:F:95:ILE:HG13	2.01	0.40
2:H:66:PRO:HB3	2:H:102:GLU:CB	2.52	0.40
1:A:306:GLU:N	1:A:306:GLU:OE2	2.38	0.40
2:H:109:PHE:CD2	2:H:133:PHE:CE1	3.09	0.40
3:L:16:TRP:CZ3	3:L:20:LYS:HD2	2.56	0.40
4:U:123:ILE:O	4:U:190:ASN:ND2	2.50	0.40
4:Y:93:MET:HG2	4:Y:131:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

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	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%)	69	82
1	C	305/454 (67%)	301 (99%)	4 (1%)	69	82
1	E	305/454 (67%)	302 (99%)	3 (1%)	76	86
1	G	305/454 (67%)	300 (98%)	5 (2%)	62	79
2	B	123/124 (99%)	123 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	123/124 (99%)	123 (100%)	0	100	100
2	F	123/124 (99%)	121 (98%)	2 (2%)	62	79
2	H	123/124 (99%)	122 (99%)	1 (1%)	81	89
3	J	32/64 (50%)	28 (88%)	4 (12%)	4	24
3	K	61/64 (95%)	60 (98%)	1 (2%)	62	79
3	L	32/64 (50%)	29 (91%)	3 (9%)	8	35
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%)	76	86
4	Y	96/133 (72%)	96 (100%)	0	100	100
All	All	2292/3100 (74%)	2264 (99%)	28 (1%)	71	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	ARG
1	A	335	SER
1	A	342	ARG
1	A	467	ASN
1	C	250	ARG
1	C	281	ASP
1	C	335	SER
1	C	467	ASN
1	E	250	ARG
1	E	281	ASP
1	E	335	SER
2	F	9	TYR
2	F	48	ASN
1	G	250	ARG
1	G	281	ASP
1	G	297	ASN
1	G	335	SER
1	G	467	ASN
2	H	92	LEU
3	K	12	ASP
3	L	10	GLN
3	L	13	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	24	ASP
4	X	147	LEU
3	J	10	GLN
3	J	14	PHE
3	J	24	ASP
3	J	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	393	GLN
1	A	496	ASN
2	B	78	GLN
2	B	110	ASN
1	C	354	HIS
1	C	467	ASN
1	C	474	HIS
2	D	78	GLN
2	D	104	ASN
2	D	110	ASN
1	E	393	GLN
1	E	496	ASN
2	F	48	ASN
2	F	55	GLN
2	F	78	GLN
2	F	110	ASN
1	G	225	GLN
1	G	241	GLN
1	G	275	ASN
1	G	297	ASN
1	G	393	GLN
1	G	467	ASN
1	G	474	HIS
2	H	55	GLN
2	H	78	GLN
2	H	104	ASN
3	K	25	GLN
3	L	10	GLN
3	L	21	GLN
3	M	40	GLN
4	U	171	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	V	121	GLN
4	V	169	HIS
4	X	188	ASN

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	339/508 (66%)	-0.15	3 (0%) 84 79	111, 210, 335, 435	0
1	C	339/508 (66%)	0.06	16 (4%) 31 27	95, 185, 348, 440	0
1	E	339/508 (66%)	-0.12	5 (1%) 73 66	118, 206, 330, 416	0
1	G	339/508 (66%)	-0.02	9 (2%) 54 45	95, 180, 323, 417	0
2	B	138/140 (98%)	0.17	3 (2%) 62 54	117, 171, 244, 269	0
2	D	138/140 (98%)	-0.02	1 (0%) 87 83	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 43	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%) 10 9	248, 306, 471, 529	0
4	U	115/153 (75%)	0.21	11 (9%) 8 7	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 7	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 34	95, 209, 364, 545	0

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	U	199	GLN	5.8
1	C	253	MET	5.6
4	U	130	LEU	5.2
4	Y	89	TYR	4.6
4	X	146	LEU	4.6
1	G	317	LEU	4.5
4	V	156	ILE	4.4
4	X	131	LYS	4.3
4	V	134	PHE	4.2
4	U	112	ALA	4.2
1	G	309	LEU	4.2
3	J	30	ALA	4.1
4	V	146	LEU	4.0
4	U	89	TYR	3.9
4	V	123	ILE	3.9
4	Y	128	ILE	3.9
1	G	232	LEU	3.8
4	X	148	ARG	3.8
4	Y	198	LEU	3.8
1	C	296	LEU	3.7
1	E	355	GLU	3.6
4	Y	146	LEU	3.5
1	G	315	LEU	3.5
1	G	253	MET	3.5
4	U	139	ASP	3.4
4	Y	130	LEU	3.4
1	C	255	ALA	3.3
3	K	69	LEU	3.3
4	V	145	THR	3.2
1	C	248	ASN	3.2
1	C	250	ARG	3.1
4	X	200	ARG	3.1
4	Y	143	THR	3.1
1	C	278	TYR	3.1
3	J	18	VAL	3.0
1	C	283	MET	3.0
1	G	250	ARG	2.9
1	C	254	ALA	2.9
4	Y	131	LYS	2.9
2	B	140	SER	2.9
1	C	270	LEU	2.8
3	J	17	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	X	130	LEU	2.8
1	C	247	LEU	2.7
1	C	271	ASN	2.7
3	M	63	GLN	2.7
3	M	29	ASP	2.7
4	X	117	VAL	2.6
1	A	349	LEU	2.6
1	C	317	LEU	2.6
3	M	32	PHE	2.6
1	C	286	ILE	2.6
1	C	272	LEU	2.6
1	A	373	CYS	2.5
1	G	270	LEU	2.5
4	Y	199	GLN	2.4
1	C	252	CYS	2.4
4	X	150	PHE	2.4
3	M	31	PRO	2.4
3	J	16	TRP	2.4
3	J	21	GLN	2.4
2	B	99	VAL	2.4
4	U	156	ILE	2.3
3	M	69	LEU	2.3
4	U	157	VAL	2.3
4	X	116	CYS	2.3
1	E	518	ILE	2.3
1	C	213	LYS	2.3
1	E	391	LEU	2.2
4	U	150	PHE	2.2
2	D	15	ARG	2.2
1	E	293	LEU	2.2
4	V	132	ALA	2.2
4	V	129	ILE	2.2
3	J	24	ASP	2.2
4	Y	134	PHE	2.2
1	E	244	ASP	2.1
3	M	26	GLU	2.1
4	Y	132	ALA	2.1
4	U	113	GLY	2.1
3	K	68	ILE	2.1
4	U	129	ILE	2.1
4	X	158	GLY	2.1
1	A	391	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	25	TYR	2.0
1	G	283	MET	2.0
1	G	296	LEU	2.0
4	X	119	MET	2.0
4	X	129	ILE	2.0
4	U	181	LEU	2.0

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.