



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:21 AM UTC

PDB ID : 6E5U / pdb_00006e5u
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

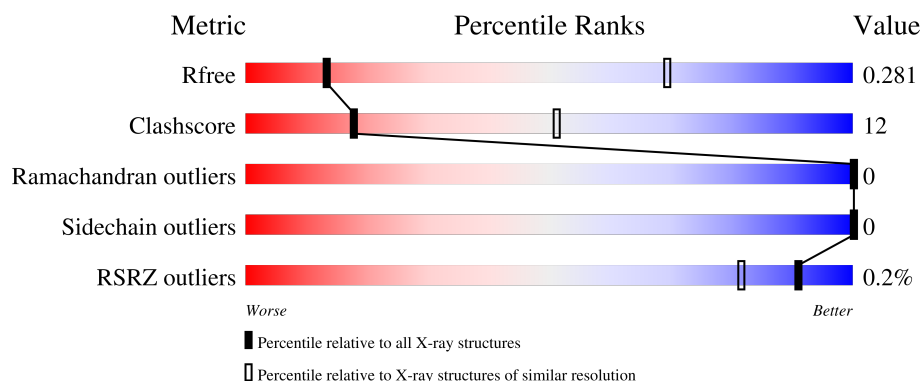
1 Overall quality at a glance

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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 of 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	 49% 18% 33%
1	C	508	 50% 17% 33%
1	E	508	 % 51% 16% 33%
1	G	508	 49% 18% 33%
2	B	140	 83% 16% .

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Mol	Chain	Length	Quality of chain
2	D	140	 71% 27%
2	F	140	 82% 16%
2	H	140	 71% 28%
3	J	77	 32% 17% 51%
3	K	77	 56% 36% 8%
3	L	77	 38% 12% 51%
3	M	77	 61% 31% 8%
4	U	153	 41% 34% 25%
4	V	153	 47% 25% 28%
4	X	153	 % 50% 25% 25%
4	Y	153	 46% 25% 28%

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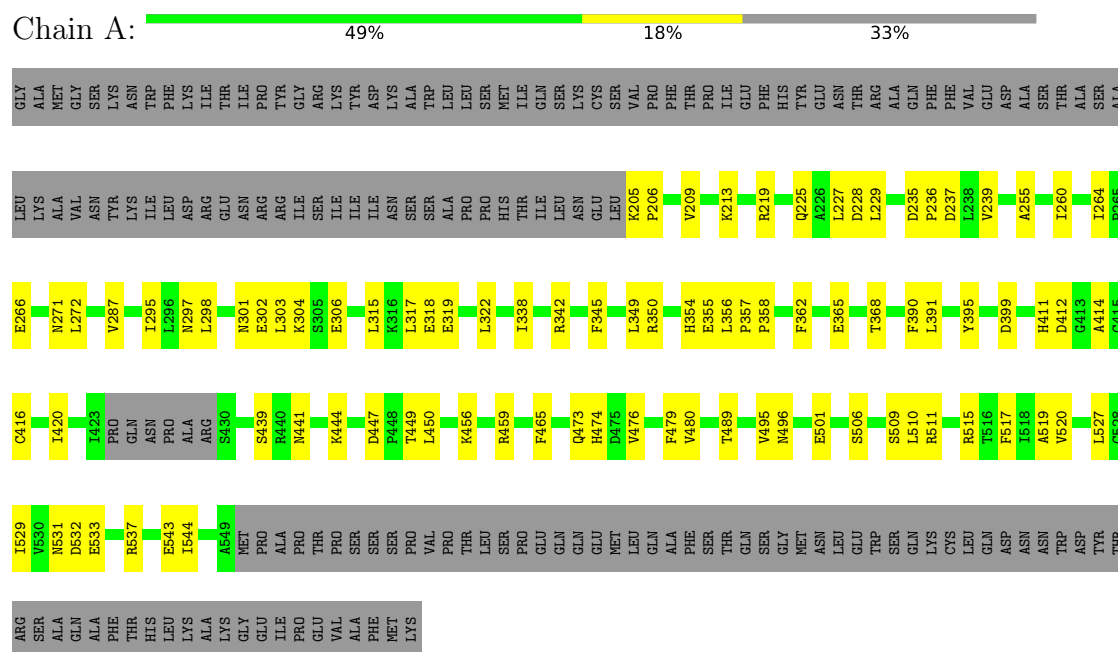
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Chain	Residue	Modelled	Actual	Comment	Reference
X	85	PRO	LEU	engineered mutation	UNP I7CAR2
Y	?	-	THR	deletion	UNP I7CAR2
Y	?	-	MET	deletion	UNP I7CAR2
Y	?	-	ALA	deletion	UNP I7CAR2
Y	?	-	SER	deletion	UNP I7CAR2
Y	?	-	ALA	deletion	UNP I7CAR2
Y	85	PRO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

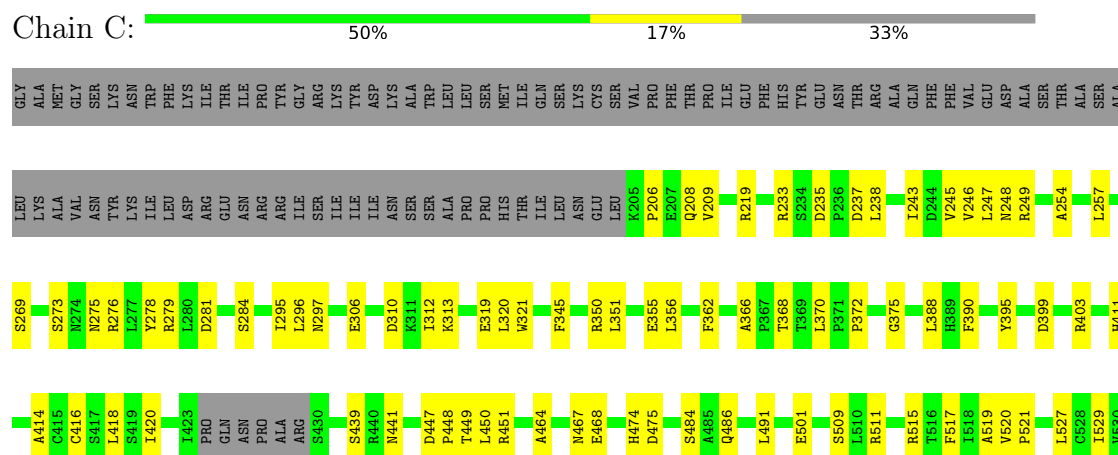
3 Residue-property plots

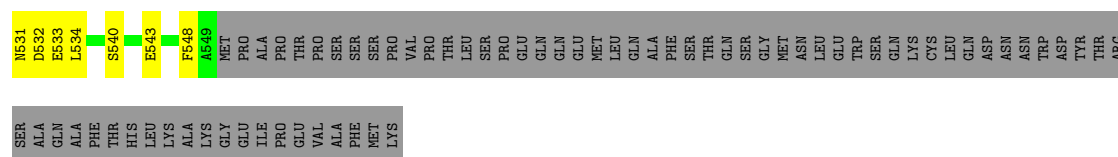
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

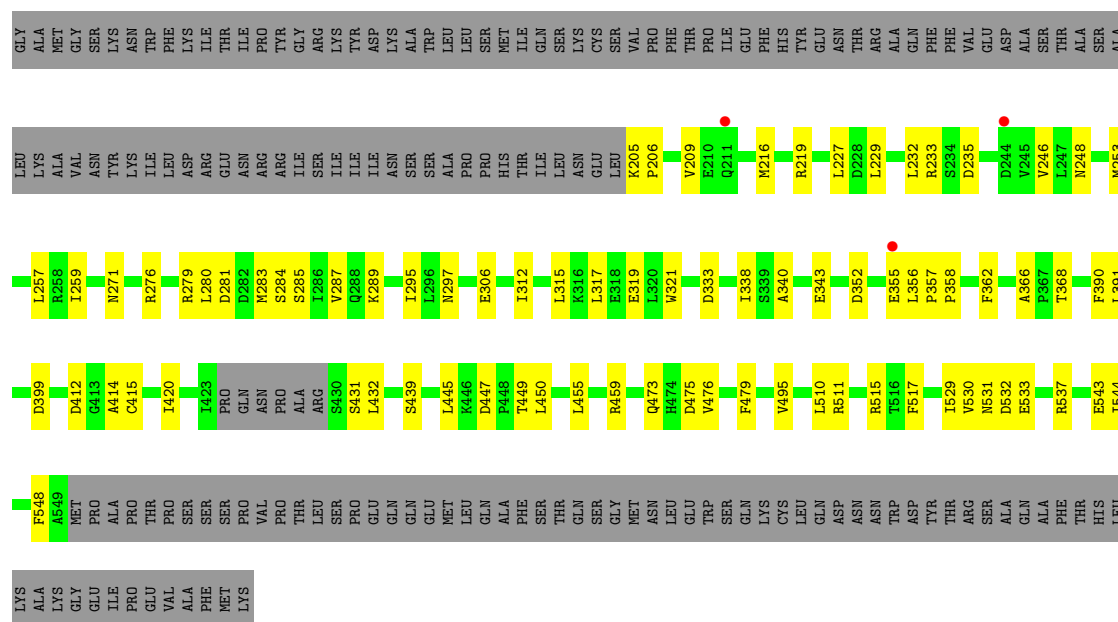


• Molecule 1: Nuclear RNA export factor 1

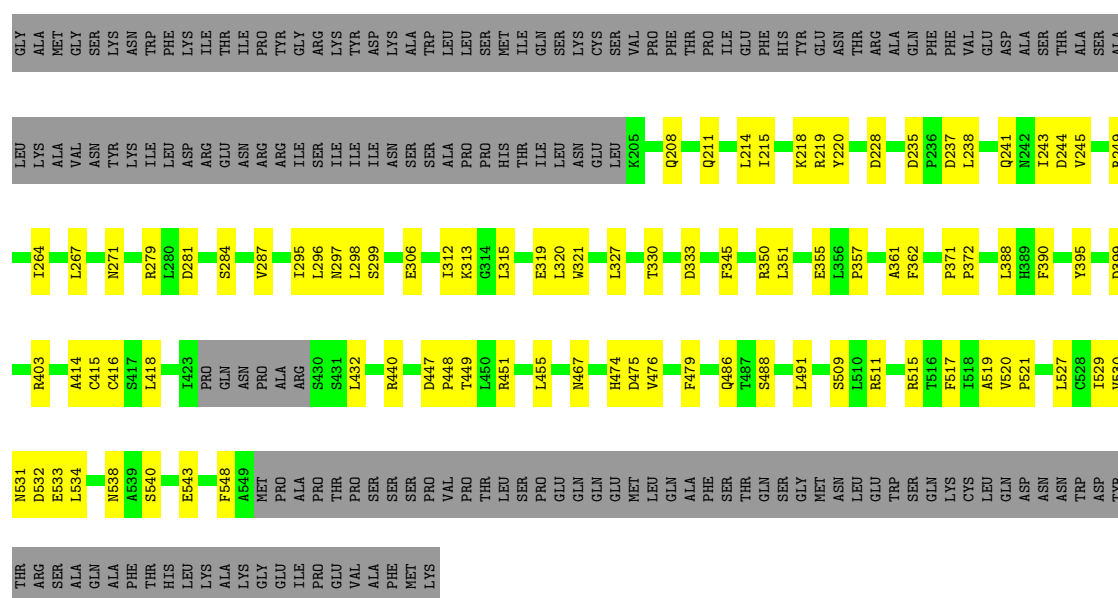




• Molecule 1: Nuclear RNA export factor 1

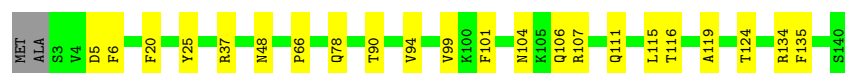


• Molecule 1: Nuclear RNA export factor 1



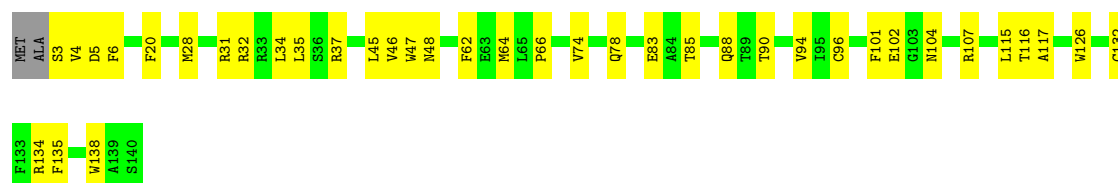
• Molecule 2: NTF2-related export protein 1

Chain B:  83% 16%



- Molecule 2: NTF2-related export protein 1

Chain D:  71% 27%



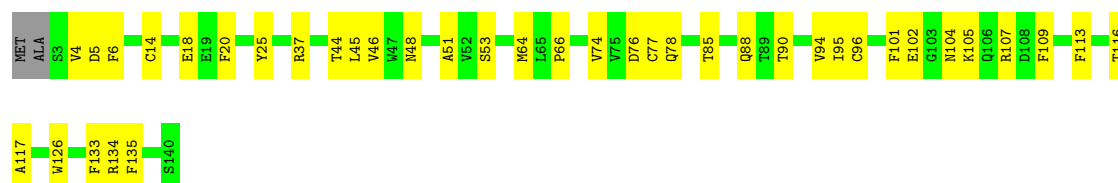
- Molecule 2: NTF2-related export protein 1

Chain F:  82% 16%



- Molecule 2: NTF2-related export protein 1

Chain H:  71% 28%



- Molecule 3: Non-structural protein 1

Chain K:  56% 36% 8%



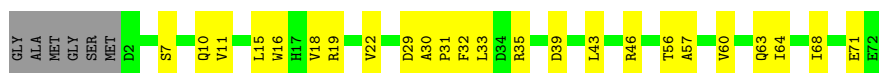
- Molecule 3: Non-structural protein 1

Chain L:  38% 12% 51%

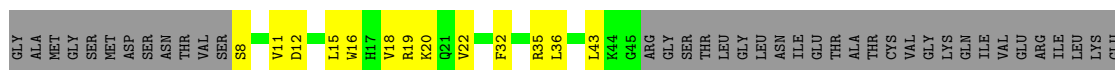
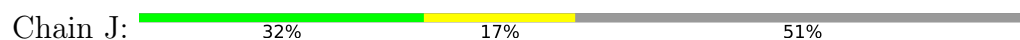


- Molecule 3: Non-structural protein 1

Chain M:  61% 31% 8%



• Molecule 3: Non-structural protein 1

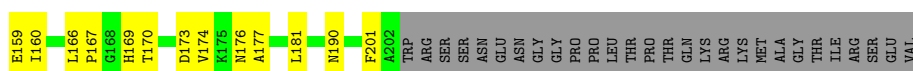


GLU

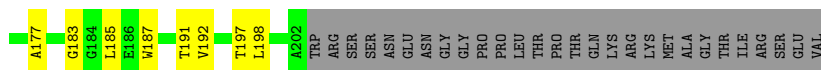
• Molecule 4: Non-structural protein 1



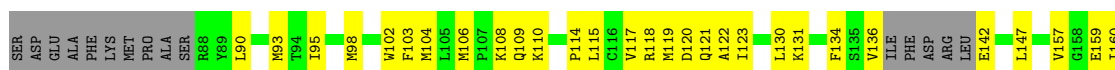
• Molecule 4: Non-structural protein 1



• Molecule 4: Non-structural protein 1



• Molecule 4: Non-structural protein 1



L166	P167	G168	H169	V174	K175	L181	M190	V194	F201	A202	TRP	ARG	SER	SER	ASN	GLU	ASN	ASN	GLY	GLY	PRO	PRO	PRO	LEU	THR	THR	PRO	THR	GLN	LYS	ARG	LYS	MET	ALA	GLY	THR	ILE	ARG	SER	GLU	VAL
------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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 , 0.281	Depositor DCC
R_{free} test set	2154 reflections (3.92%)	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)	0.32 , 428.9	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	0.91	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 [i](#)

5.1 Standard geometry [i](#)

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	0.25	1/2738 (0.0%)	0.50	0/3699
1	C	0.26	0/2738	0.53	0/3699
1	E	0.25	1/2738 (0.0%)	0.49	0/3699
1	G	0.25	0/2738	0.54	0/3699
2	B	0.27	0/1123	0.51	0/1524
2	D	0.30	0/1123	0.55	0/1524
2	F	0.25	0/1123	0.49	0/1524
2	H	0.29	0/1123	0.54	0/1524
3	J	0.39	0/313	0.63	0/421
3	K	0.21	0/560	0.46	0/754
3	L	0.20	0/313	0.42	0/421
3	M	0.21	0/560	0.44	0/754
4	U	0.21	0/924	0.53	0/1250
4	V	0.24	0/876	0.56	0/1184
4	X	0.21	0/924	0.52	0/1250
4	Y	0.23	0/876	0.53	0/1184
All	All	0.25	2/20790 (0.0%)	0.52	0/28110

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	358	PRO	CA-C	-6.00	1.48	1.51
1	A	358	PRO	CA-C	-5.43	1.48	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2693	0	2724	58	0
1	C	2693	0	2724	68	0
1	E	2693	0	2724	52	0
1	G	2693	0	2724	71	0
2	B	1099	0	1050	16	0
2	D	1099	0	1050	33	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	25	0
4	U	909	0	923	40	0
4	V	863	0	874	33	0
4	X	909	0	923	31	0
4	Y	863	0	874	30	0
All	All	20434	0	20384	500	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 (500) 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

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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
4:Y:93:MET:HB2	4:Y:98:MET:HE2	1.78	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:533:GLU:HG2	2:F:94:VAL:HG21	1.80	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:95:ILE:HA	4:Y:98:MET:HB2	1.86	0.58
1:C:416:CYS:HA	1:C:532:ASP:O	2.03	0.58
1:C:520:VAL:HG13	1:C:521:PRO:HD2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ASP:HA	1:E:459:ARG:HD2	1.88	0.55
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:48:ASN:ND2	2:B:134:ARG:HA	2.24	0.53
2:B:119:ALA:HA	2:B:124:THR:HG22	1.89	0.53
3:K:53:ASN:O	3:K:56:THR:OG1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:418:LEU:HD12	1:C:534:LEU:O	2.09	0.52
1:A:225:GLN:NE2	1:A:266:GLU:HG2	2.23	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
4:Y:108:LYS:HB3	4:Y:110:LYS:HZ2	1.75	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
1:G:297:ASN:HD22	1:G:297:ASN:C	2.19	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:NZ	1:G:218:LYS:HB3	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
4:X:102:TRP:CZ3	4:X:104:MET:HE2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:306:GLU:H	1:G:306:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:362:PHE:CZ	2:D:20:PHE:HB2	2.48	0.47
1:C:411:HIS:H	1:C:414:ALA:HB2	1.78	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: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
3:J:32:PHE:CE2	3:J:35:ARG:NH2	2.82	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:X:102:TRP:HZ3	4:X:104:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:521:PRO:HD3	4:Y:103:PHE:CE2	2.50	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: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:OD1	1:E:333:ASP:N	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
4:U:133:ASN:O	4:U:145:THR:OG1	2.19	0.46
4:V:108:LYS:HE2	4:V:110:LYS:HZ3	1.79	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:14:CYS:O	2:H:18:GLU:HG2	2.16	0.46
2:H:48:ASN:ND2	2:H:134:ARG:HA	2.31	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
1:E:216:MET:HE3	1:E:227:LEU:HD21	1.98	0.46
2:H:109:PHE:CD2	2:H:133:PHE:HE1	2.33	0.46
4:U:104:MET:HE1	4:U:118:ARG:HB3	1.98	0.46
4:X:128:ILE:O	4:X:192:VAL:HA	2.16	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:X:98:MET:HE1	4:X:146:LEU:HB2	1.98	0.45
2:D:74:VAL:CG2	2:D:96:CYS:HB3	2.47	0.45
2:H:37:ARG:HA	2:H:37:ARG:HD3	1.79	0.45
4:V:125:ASP:N	4:V:190:ASN:OD1	2.49	0.45
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
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
3:J:18:VAL:O	3:J:22:VAL:HG23	2.18	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:114:PRO:HG3	4:V:167:PRO:HD2	1.98	0.44
4:V:132:ALA:HB2	4:V:147:LEU:HD23	1.98	0.44
1:A:298:LEU:HB3	1:A:303:LEU:HD11	1.98	0.44
2:F:5:ASP:OD1	2:F:6:PHE:N	2.50	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:K:63:GLN:NE2	4:X:197:THR:HG22	2.26	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
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: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
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
1:E:315:LEU:HD13	1:E:317:LEU:HD21	1.99	0.43
2:F:38:LEU:HD23	2:F:38:LEU:HA	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
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: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
3:J:16:TRP:CZ3	3:J:20:LYS:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:U:149:ALA:O	4:U:156:ILE:HA	2.19	0.42
3:J:32:PHE:HE2	3:J:35:ARG:HH21	1.67	0.42
1:A:354:HIS:HA	2:D:3:SER:O	2.19	0.42
1:C:484:SER:OG	2:D:132:CYS:HB2	2.20	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:HD3	2:B:37:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:V:102:TRP:CZ3	4:V:104:MET:HE2	2.55	0.41
4:Y:136:VAL:C	4:Y:142:GLU:HG3	2.46	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:362:PHE:CE1	2:H:126:TRP:HB2	2.56	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
4:U:89:TYR:CD1	4:U:135:SER:HB3	2.56	0.41
1:C:370:LEU:HD11	2:D:104:ASN:CG	2.46	0.40
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:OE2	1:A:306:GLU:N	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

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%)	305 (100%)	0	100	100
1	C	305/454 (67%)	305 (100%)	0	100	100
1	E	305/454 (67%)	305 (100%)	0	100	100
1	G	305/454 (67%)	305 (100%)	0	100	100
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%)	123 (100%)	0	100	100
2	H	123/124 (99%)	123 (100%)	0	100	100
3	J	32/64 (50%)	32 (100%)	0	100	100
3	K	61/64 (95%)	61 (100%)	0	100	100
3	L	32/64 (50%)	32 (100%)	0	100	100
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%)	101 (100%)	0	100	100
4	Y	96/133 (72%)	96 (100%)	0	100	100
All	All	2292/3100 (74%)	2292 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	275	ASN
1	A	382	ASN
1	A	393	GLN
1	A	496	ASN
2	B	78	GLN
2	B	81	HIS
2	B	88	GLN
1	C	334	GLN
1	C	354	HIS
1	C	382	ASN
1	C	461	ASN
1	C	467	ASN
1	C	474	HIS

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Mol	Chain	Res	Type
1	C	496	ASN
2	D	50	ASN
2	D	78	GLN
2	D	88	GLN
2	D	106	GLN
2	D	110	ASN
1	E	292	ASN
1	E	334	GLN
1	E	393	GLN
1	E	461	ASN
1	E	467	ASN
1	E	496	ASN
1	E	531	ASN
2	F	48	ASN
2	F	78	GLN
2	F	88	GLN
2	F	106	GLN
2	F	110	ASN
1	G	241	GLN
1	G	297	ASN
1	G	334	GLN
1	G	354	HIS
1	G	393	GLN
1	G	461	ASN
1	G	467	ASN
1	G	474	HIS
1	G	496	ASN
2	H	55	GLN
2	H	78	GLN
2	H	104	ASN
2	H	106	GLN
2	H	110	ASN
3	K	25	GLN
3	L	10	GLN
3	L	21	GLN
3	L	25	GLN
3	M	40	GLN
3	M	63	GLN
4	U	171	ASN
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 oligosaccharides 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%)	-0.57	0	100	100	111, 210, 335, 435	0
1	C	339/508 (66%)	-0.61	0	100	100	95, 185, 348, 440	0
1	E	339/508 (66%)	-0.55	3 (0%)	81	60	118, 206, 330, 416	0
1	G	339/508 (66%)	-0.65	0	100	100	95, 180, 323, 417	0
2	B	138/140 (98%)	-0.48	0	100	100	117, 171, 244, 269	0
2	D	138/140 (98%)	-0.71	0	100	100	101, 143, 245, 310	0
2	F	138/140 (98%)	-0.61	0	100	100	106, 160, 225, 264	0
2	H	138/140 (98%)	-0.62	0	100	100	104, 145, 246, 325	0
3	J	38/77 (49%)	-0.18	0	100	100	290, 387, 487, 545	0
3	K	71/77 (92%)	-0.49	0	100	100	194, 261, 383, 401	0
3	L	38/77 (49%)	-0.39	0	100	100	248, 318, 419, 435	0
3	M	71/77 (92%)	-0.10	0	100	100	248, 306, 471, 529	0
4	U	115/153 (75%)	-0.50	0	100	100	193, 256, 338, 408	0
4	V	110/153 (71%)	-0.28	0	100	100	177, 307, 400, 487	0
4	X	115/153 (75%)	-0.49	1 (0%)	81	60	192, 256, 341, 412	0
4	Y	110/153 (71%)	-0.46	0	100	100	162, 301, 378, 420	0
All	All	2576/3512 (73%)	-0.54	4 (0%)	91	81	95, 209, 364, 545	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	355	GLU	2.7
1	E	211	GLN	2.4
4	X	145	THR	2.1
1	E	244	ASP	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 oligosaccharides 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.