wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 01:17 PM EST

PDB ID	:	2G9T
Title	:	Crystal structure of the SARS coronavirus nsp10 at 2.1A
Authors	:	Su, D.; Lou, Z.; Yang, H.; Sun, F.; Rao, Z.
Deposited on	:	2006-03-07
Resolution	:	2.10 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 (i) 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 (1)) were used in the production of this report:

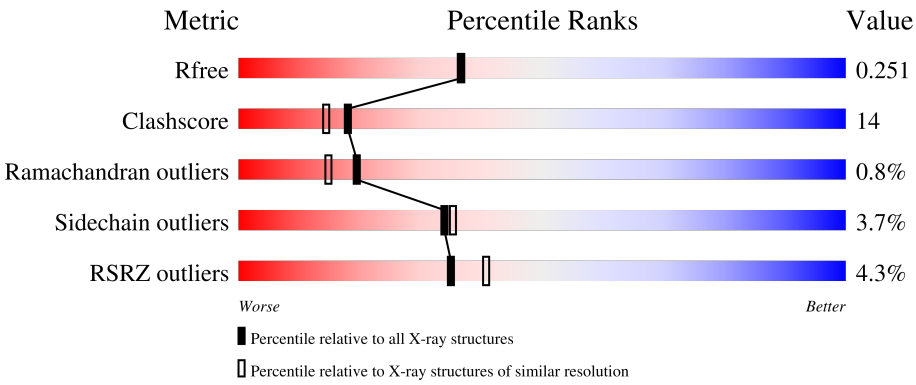
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	152	% 72% 5% • 22%
1	B	152	3% 65% 10% • 22%
1	C	152	3% 60% 16% • 22%
1	D	152	4% 55% 19% • 22%
1	E	152	3% 56% 18% • • 22%

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Mol	Chain	Length	Quality of chain
1	F	152	3% 61% 15% 23%
1	G	152	4% 61% 12% 22%
1	H	152	5% 68% 7% 22%
1	I	152	3% 62% 14% 22%
1	J	152	3% 61% 16% 22%
1	K	152	2% 59% 16% 22%
1	L	152	3% 65% 9% 22%
1	M	152	3% 56% 18% 22%
1	N	152	4% 66% 11% 22%
1	O	152	5% 58% 18% 22%
1	P	152	3% 65% 10% 22%
1	Q	152	3% 60% 16% 22%
1	R	152	2% 61% 14% 22%
1	S	152	3% 65% 9% 22%
1	T	152	5% 62% 12% 22%
1	U	152	5% 62% 12% 24%
1	V	152	5% 59% 14% 24%
1	W	152	3% 65% 11% 22%
1	X	152	5% 56% 19% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22470 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 orf1a polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	873	544	147	167	15	0	0	0
1	B	119	880	549	148	168	15	0	0	0
1	C	118	873	544	147	167	15	0	0	0
1	D	118	873	544	147	167	15	0	0	0
1	E	118	873	544	147	167	15	0	0	0
1	F	117	863	538	144	166	15	0	0	0
1	G	118	873	544	147	167	15	0	0	0
1	H	118	873	544	147	167	15	0	0	0
1	I	118	873	544	147	167	15	0	0	0
1	J	118	873	544	147	167	15	0	0	0
1	K	118	873	544	147	167	15	0	0	0
1	L	118	873	544	147	167	15	0	0	0
1	M	118	873	544	147	167	15	0	0	0
1	N	118	873	544	147	167	15	0	0	0
1	O	118	873	544	147	167	15	0	0	0
1	P	118	873	544	147	167	15	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	118	873	544	147	167	15	0	0	0
1	R	118	873	544	147	167	15	0	0	0
1	S	118	873	544	147	167	15	0	0	0
1	T	118	873	544	147	167	15	0	0	0
1	U	116	856	534	143	164	15	0	0	0
1	V	116	856	534	143	164	15	0	0	0
1	W	118	873	544	147	167	15	0	0	0
1	X	118	873	544	147	167	15	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0
2	I	2	2	2	0	0
2	J	2	2	2	0	0
2	K	2	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	2	Total Zn 2 2	0	0
2	M	2	Total Zn 2 2	0	0
2	N	2	Total Zn 2 2	0	0
2	O	2	Total Zn 2 2	0	0
2	P	2	Total Zn 2 2	0	0
2	Q	2	Total Zn 2 2	0	0
2	R	2	Total Zn 2 2	0	0
2	S	2	Total Zn 2 2	0	0
2	T	2	Total Zn 2 2	0	0
2	U	2	Total Zn 2 2	0	0
2	V	2	Total Zn 2 2	0	0
2	W	2	Total Zn 2 2	0	0
2	X	2	Total Zn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	59	Total O 59 59	0	0
3	C	66	Total O 66 66	0	0
3	D	63	Total O 63 63	0	0
3	E	63	Total O 63 63	0	0
3	F	58	Total O 58 58	0	0

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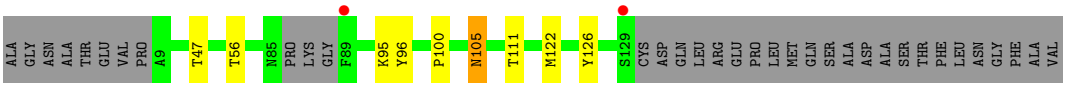
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	65	Total O 65 65	0	0
3	H	59	Total O 59 59	0	0
3	I	55	Total O 55 55	0	0
3	J	73	Total O 73 73	0	0
3	K	71	Total O 71 71	0	0
3	L	71	Total O 71 71	0	0
3	M	74	Total O 74 74	0	0
3	N	51	Total O 51 51	0	0
3	O	45	Total O 45 45	0	0
3	P	58	Total O 58 58	0	0
3	Q	81	Total O 81 81	0	0
3	R	61	Total O 61 61	0	0
3	S	67	Total O 67 67	0	0
3	T	62	Total O 62 62	0	0
3	U	77	Total O 77 77	0	0
3	V	49	Total O 49 49	0	0
3	W	45	Total O 45 45	0	0
3	X	65	Total O 65 65	0	0

3 Residue-property plots (i)

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.

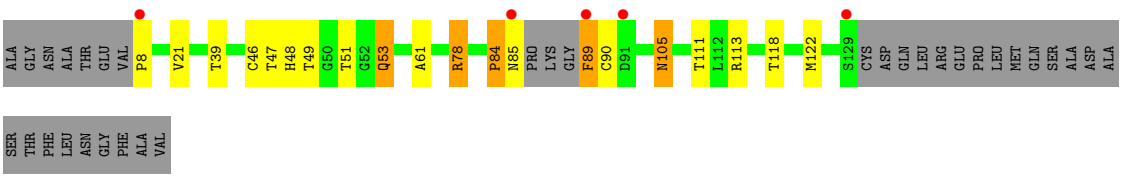
• Molecule 1: orf1a polyprotein

Chain A:



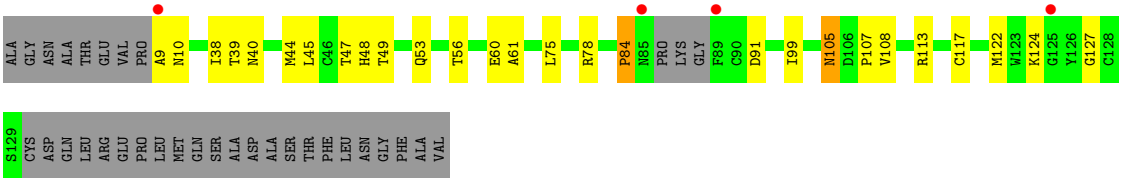
• Molecule 1: orf1a polyprotein

Chain B:



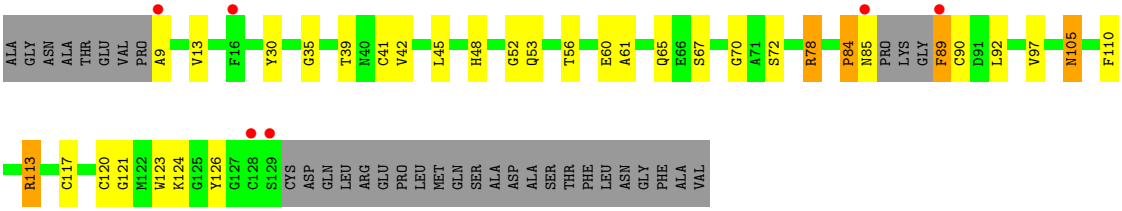
• Molecule 1: orf1a polyprotein

Chain C:



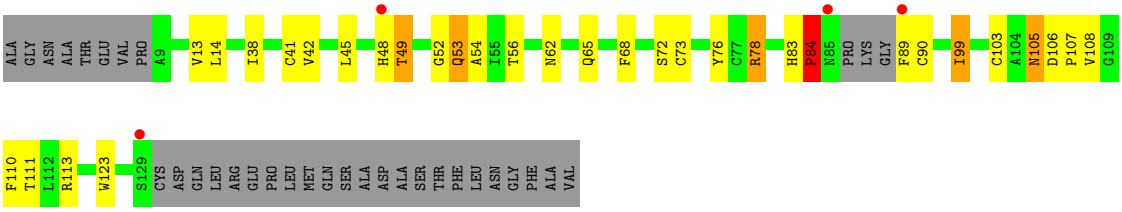
• Molecule 1: orf1a polyprotein

Chain D:



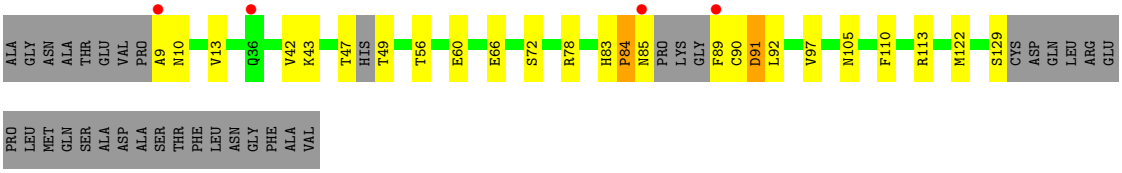
• Molecule 1: orf1a polyprotein

Chain E:



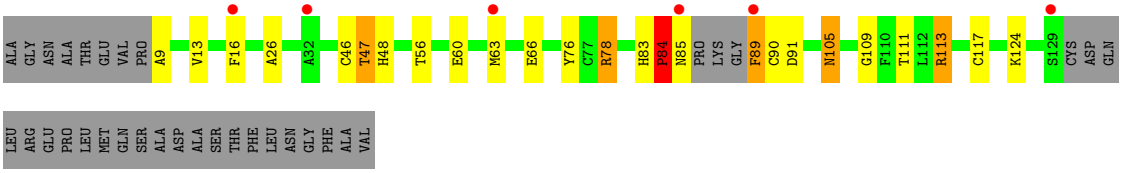
• Molecule 1: orf1a polyprotein

Chain F:



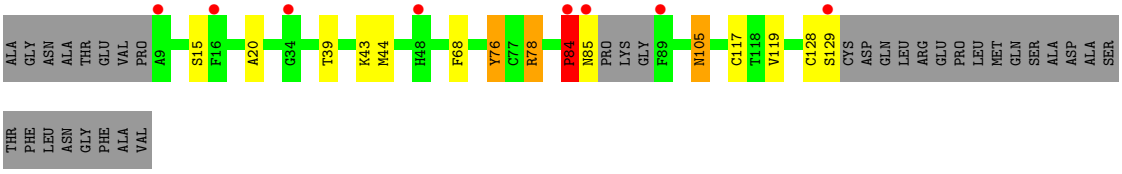
• Molecule 1: orf1a polyprotein

Chain G:



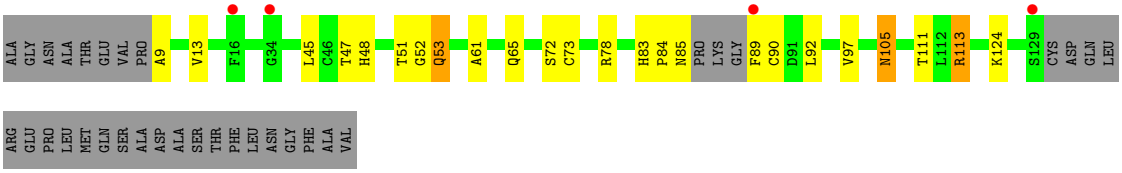
• Molecule 1: orf1a polyprotein

Chain H:



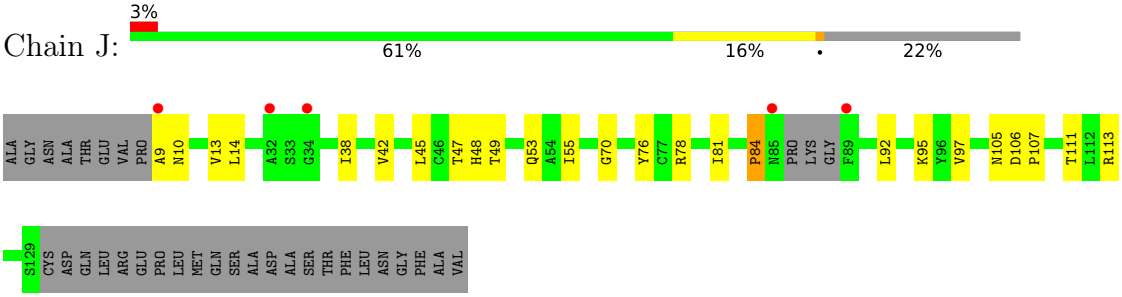
• Molecule 1: orf1a polyprotein

Chain I:



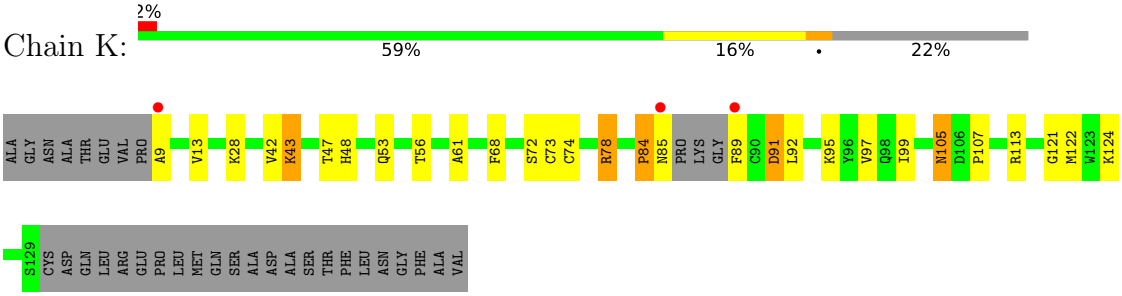
• Molecule 1: orf1a polyprotein

Chain J:



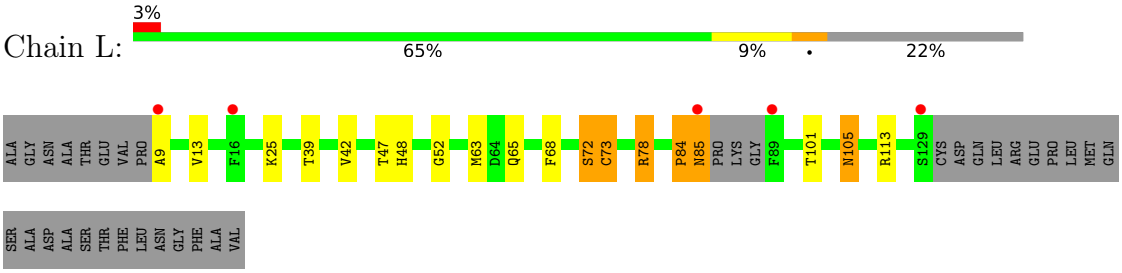
• Molecule 1: orf1a polyprotein

Chain K:



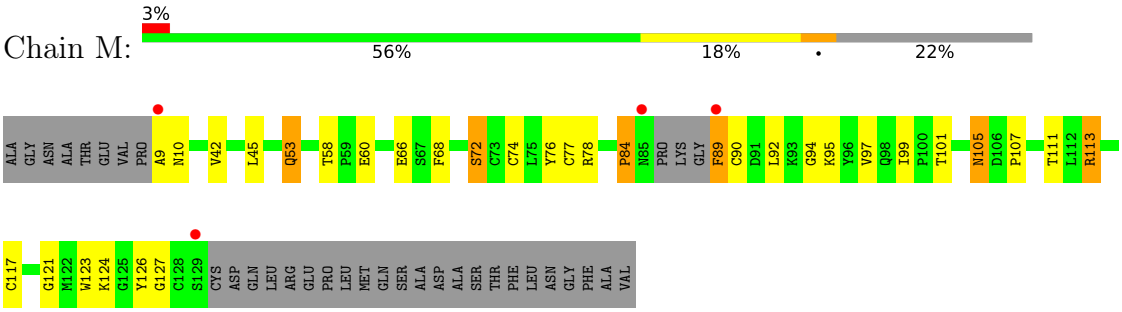
• Molecule 1: orf1a polyprotein

Chain L:



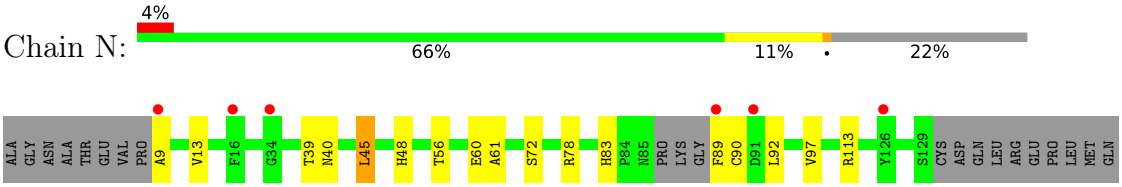
• Molecule 1: orf1a polyprotein

Chain M:



• Molecule 1: orf1a polyprotein

Chain N:



SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL

- Molecule 1: orf1a polyprotein

Chain O: 5% 58% 18% • 22%

ALA GLY ASN ALA THR GLU VAL PRO A9 V13 F16 Y30 G34 G35 Q36 P37 I38 V42 T47 H48 T49 G52 I55 S72 R78 C79 H80 H83 P84 N85 PRO LYS GLY F89 C90 D91 L92 K95 Y96 I99 D106 P107 V108 T111 L112

R113 M122 G125 Y126 S129 CYS ASP GLN LEU ARG GLU PRO LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL

- Molecule 1: orf1a polyprotein

Chain P: 3% 65% 10% • 22%

ALA GLY ASN ALA THR GLU VAL PRO A9 L14 S15 F16 V42 K43 M44 L45 A54 I55 G69 S72 R78 P84 N85 PRO LYS GLY F89 K95 I99 N105 D106 P107 F110 T111 L112 R113 W123 Y126 S129 CYS ASP GLN LEU ARG GLU PRO

LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL

- Molecule 1: orf1a polyprotein

Chain Q: 3% 60% 16% • 22%

ALA GLY ASN ALA THR GLU VAL PRO A9 V13 Q36 V42 K43 M44 L45 C46 T47 H48 Q53 A61 F68 G69 S72 C73 Y76 C77 R78 H83 P84 N85 PRO LYS GLY F89 C90 I99 N105 T111 L112 R113 K124 C128 S129 CYS ASP GLN

LEU ARG GLU PRO LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL

- Molecule 1: orf1a polyprotein

Chain R: 2% 61% 14% • 22%

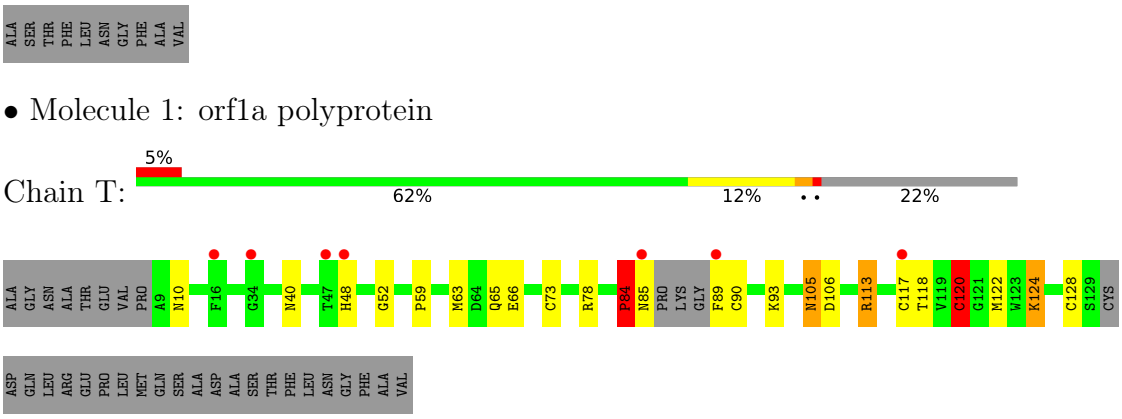
ALA GLY ASN ALA THR GLU VAL PRO A9 T39 M44 L45 H48 T51 Q52 Q53 T56 E60 A61 E66 S72 R78 H83 P84 N85 PRO LYS GLY F89 C90 D91 Q98 I99 P100 T101 N105 R113 W123 Y126 S129 CYS ASP GLN LEU

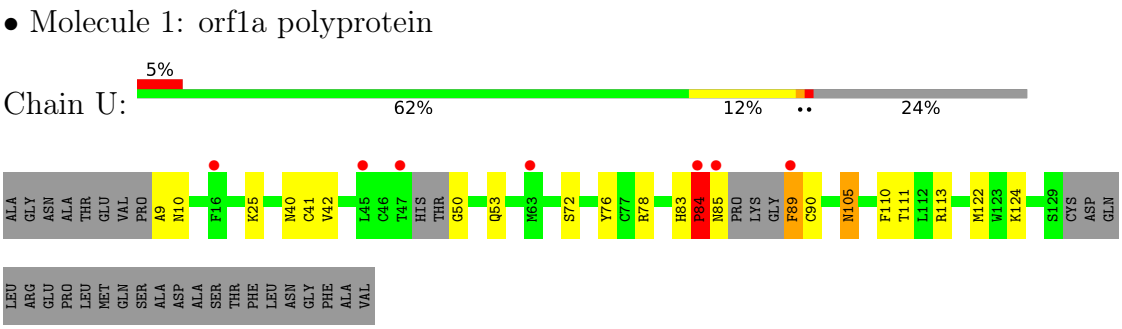
ARG GLU PRO LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL

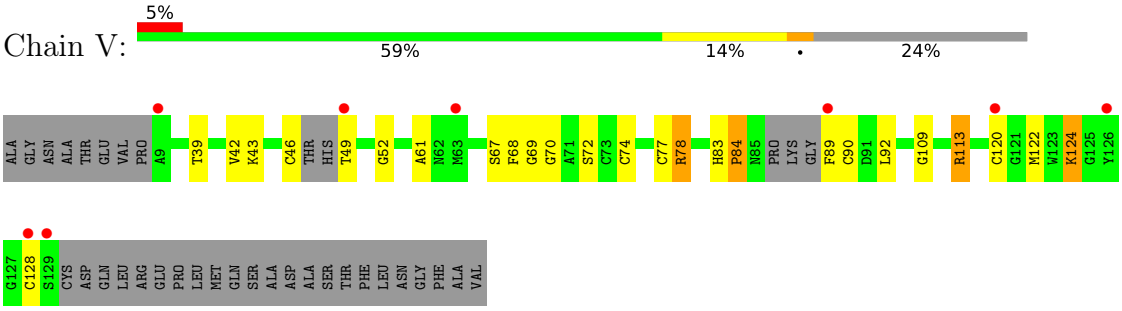
- Molecule 1: orf1a polyprotein

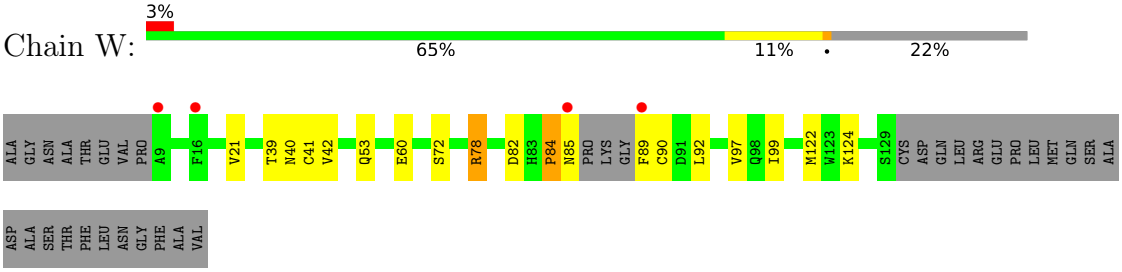
Chain S: 3% 65% 9% • • 22%

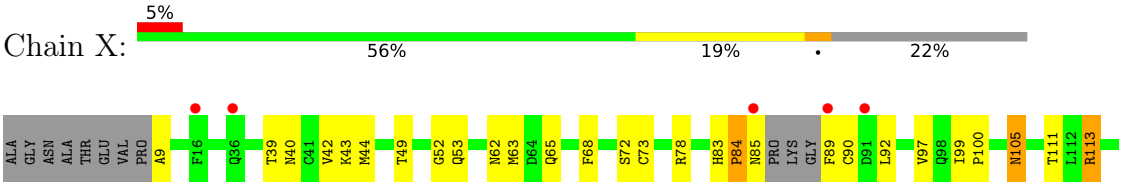
ALA GLY ASN ALA THR GLU VAL PRO A9 K25 N40 K43 M44 L45 C46 Q53 E66 S72 R78 H83 P84 N85 PRO LYS GLY F89 C90 I99 N105 D106 P107 T111 K124 S129 CYS ASP GLN LEU ARG GLU PRO LEU MET GLN SER ALA ASP

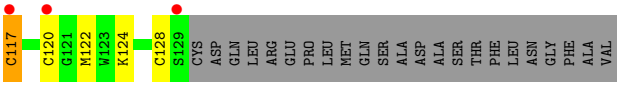

ALA SER THR PHE LEU ASN GLY PHE ALA VAL
• Molecule 1: orf1a polyprotein
Chain T:
5%
62%
12%
22%
ALA GLY ASN ALA THR GLU VAL PRO A9 N10 F16 G34 N40 T47 H48 G52 P59 M63 D64 Q65 E66 C73 R78 P84 N85 PRO LYS GLY F89 C90 K93 N105 D106 R113 C117 T118 V119 C120 G121 M122 W123 K124 C128 S129 CYS
ASP GLN LEU ARG GLU PRO LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL


• Molecule 1: orf1a polyprotein
Chain U:
5%
62%
12%
24%
ALA GLY ASN ALA THR GLU VAL PRO A9 N10 F16 K25 N40 C41 V42 L45 C46 T47 HIS THR G50 Q53 M63 S72 Y76 C77 R78 H83 P84 N85 PRO LYS GLY F89 C90 N105 F110 T111 L112 R113 M122 W123 K124 S129 CYS ASP GLN
LEU ARG GLU PRO LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL


• Molecule 1: orf1a polyprotein
Chain V:
5%
59%
14%
24%
ALA GLY ASN ALA THR GLU VAL PRO A9 T39 V42 K43 C46 THR HIS T49 G52 A61 N62 M63 S67 F68 G69 G70 A71 S72 C73 C74 C77 R78 H83 P84 N85 PRO LYS GLY F89 C90 D91 L92 G109 R113 C120 G121 M122 W123 K124 G125 Y126
G127 C128 S129 CYS ASP GLN LEU ARG GLU PRO LEU MET GLN SER ALA ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL


• Molecule 1: orf1a polyprotein
Chain W:
3%
65%
11%
22%
ALA GLY ASN ALA THR GLU VAL PRO A9 F16 V21 T39 N40 C41 V42 Q53 E60 S72 R78 D82 H83 P84 N85 PRO LYS GLY F89 C90 D91 L92 V97 Q98 I99 M122 W123 K124 S129 CYS ASP GLN LEU ARG GLU PRO LEU MET GLN SER ALA
ASP ALA SER THR PHE LEU ASN GLY PHE ALA VAL


• Molecule 1: orf1a polyprotein
Chain X:
5%
56%
19%
22%
ALA GLY ASN ALA THR GLU VAL PRO A9 F16 Q36 T39 N40 C41 V42 K43 M44 T49 G52 Q53 N62 M63 D64 Q65 F68 S72 C73 R78 H83 P84 N85 PRO LYS GLY F89 C90 D91 L92 V97 Q98 I99 P100 N105 T111 L112 R113


C117
C120
G121
M122
W123
K124
C128
S129
CYS
ASP
GLN
LEU
ARG
GLU
PRO
LEU
MET
GLN
SER
ALA
ASP
ALA
SER
THR
PHE
LEU
ASN
GLY
PHE
ALA
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	159.11Å 321.83Å 161.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 97.4 (49.80-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.247 0.221 , 0.251	Depositor DCC
R_{free} test set	25972 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22470	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.65	0/892	0.82	1/1211 (0.1%)
1	B	0.63	0/900	0.82	1/1222 (0.1%)
1	C	0.61	0/892	0.84	3/1211 (0.2%)
1	D	0.63	0/892	0.86	2/1211 (0.2%)
1	E	0.68	1/892 (0.1%)	0.82	1/1211 (0.1%)
1	F	0.60	0/880	0.79	1/1193 (0.1%)
1	G	0.66	1/892 (0.1%)	0.90	3/1211 (0.2%)
1	H	0.62	0/892	0.81	1/1211 (0.1%)
1	I	0.66	0/892	0.87	3/1211 (0.2%)
1	J	0.65	0/892	0.87	3/1211 (0.2%)
1	K	0.61	0/892	0.89	2/1211 (0.2%)
1	L	0.67	1/892 (0.1%)	0.86	1/1211 (0.1%)
1	M	0.66	0/892	0.89	3/1211 (0.2%)
1	N	0.58	0/892	0.79	1/1211 (0.1%)
1	O	0.57	0/892	0.77	1/1211 (0.1%)
1	P	0.61	0/892	0.78	0/1211
1	Q	0.67	0/892	0.83	2/1211 (0.2%)
1	R	0.64	0/892	0.82	1/1211 (0.1%)
1	S	0.64	1/892 (0.1%)	0.77	0/1211
1	T	0.70	1/892 (0.1%)	0.86	2/1211 (0.2%)
1	U	0.64	0/873	0.84	2/1183 (0.2%)
1	V	0.60	0/873	0.83	2/1183 (0.2%)
1	W	0.62	0/892	0.88	2/1211 (0.2%)
1	X	0.68	0/892	0.95	5/1211 (0.4%)
All	All	0.64	5/21366 (0.0%)	0.84	43/29001 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	120	CYS	CB-SG	-9.17	1.66	1.82
1	E	73	CYS	CB-SG	-8.22	1.68	1.82
1	S	46	CYS	CB-SG	7.25	1.94	1.82
1	L	73	CYS	CB-SG	-6.80	1.70	1.82
1	G	46	CYS	CB-SG	5.68	1.92	1.82

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	78	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	I	78	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	G	78	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	W	78	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	M	78	ARG	NE-CZ-NH2	-10.17	115.21	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	TYR	Sidechain
1	E	76	TYR	Sidechain
1	G	76	TYR	Sidechain
1	H	76	TYR	Sidechain
1	M	76	TYR	Sidechain

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	873	0	829	7	0
1	B	880	0	837	19	0
1	C	873	0	829	27	0
1	D	873	0	829	37	0
1	E	873	0	829	30	0
1	F	863	0	821	30	0
1	G	873	0	829	27	0
1	H	873	0	829	13	0
1	I	873	0	829	21	0
1	J	873	0	829	20	0
1	K	873	0	829	30	0
1	L	873	0	829	19	0
1	M	873	0	829	32	0
1	N	873	0	829	10	0
1	O	873	0	829	23	0
1	P	873	0	829	25	0
1	Q	873	0	829	26	0
1	R	873	0	829	23	0
1	S	873	0	829	30	0
1	T	873	0	829	33	0
1	U	856	0	814	26	0
1	V	856	0	814	17	0
1	W	873	0	829	14	0
1	X	873	0	829	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
3	A	69	0	0	4	0
3	B	59	0	0	4	0
3	C	66	0	0	5	0
3	D	63	0	0	4	0
3	E	63	0	0	8	0
3	F	58	0	0	6	0
3	G	65	0	0	12	0
3	H	59	0	0	2	0
3	I	55	0	0	8	0
3	J	73	0	0	5	0
3	K	71	0	0	15	0
3	L	71	0	0	0	0
3	M	74	0	0	11	0
3	N	51	0	0	1	0
3	O	45	0	0	7	0
3	P	58	0	0	11	0
3	Q	81	0	0	8	0
3	R	61	0	0	9	0
3	S	67	0	0	13	0
3	T	62	0	0	10	0
3	U	77	0	0	13	0
3	V	49	0	0	6	0
3	W	45	0	0	0	0
3	X	65	0	0	10	0
All	All	22470	0	19866	552	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 14.

The worst 5 of 552 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:THR:HG23	1:B:49:THR:H	1.14	1.08
1:P:14:LEU:HD11	1:P:78:ARG:HH12	1.22	1.00
1:S:72:SER:HB3	3:S:1026:HOH:O	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:43:LYS:HD3	3:Q:1031:HOH:O	1.63	0.99
1:S:40:ASN:HB2	1:S:78:ARG:HH22	1.32	0.94

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	114/152 (75%)	110 (96%)	4 (4%)	0	100	100
1	B	115/152 (76%)	109 (95%)	5 (4%)	1 (1%)	17	12
1	C	114/152 (75%)	110 (96%)	3 (3%)	1 (1%)	17	12
1	D	114/152 (75%)	109 (96%)	4 (4%)	1 (1%)	17	12
1	E	114/152 (75%)	107 (94%)	5 (4%)	2 (2%)	8	4
1	F	111/152 (73%)	104 (94%)	6 (5%)	1 (1%)	17	12
1	G	114/152 (75%)	109 (96%)	4 (4%)	1 (1%)	17	12
1	H	114/152 (75%)	107 (94%)	6 (5%)	1 (1%)	17	12
1	I	114/152 (75%)	107 (94%)	7 (6%)	0	100	100
1	J	114/152 (75%)	111 (97%)	3 (3%)	0	100	100
1	K	114/152 (75%)	107 (94%)	6 (5%)	1 (1%)	17	12
1	L	114/152 (75%)	110 (96%)	3 (3%)	1 (1%)	17	12
1	M	114/152 (75%)	110 (96%)	2 (2%)	2 (2%)	8	4
1	N	114/152 (75%)	110 (96%)	4 (4%)	0	100	100
1	O	114/152 (75%)	105 (92%)	8 (7%)	1 (1%)	17	12
1	P	114/152 (75%)	107 (94%)	6 (5%)	1 (1%)	17	12
1	Q	114/152 (75%)	109 (96%)	4 (4%)	1 (1%)	17	12
1	R	114/152 (75%)	110 (96%)	3 (3%)	1 (1%)	17	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	114/152 (75%)	108 (95%)	5 (4%)	1 (1%)	17	12
1	T	114/152 (75%)	110 (96%)	3 (3%)	1 (1%)	17	12
1	U	110/152 (72%)	105 (96%)	4 (4%)	1 (1%)	17	12
1	V	110/152 (72%)	103 (94%)	6 (6%)	1 (1%)	17	12
1	W	114/152 (75%)	109 (96%)	4 (4%)	1 (1%)	17	12
1	X	114/152 (75%)	109 (96%)	4 (4%)	1 (1%)	17	12
All	All	2726/3648 (75%)	2595 (95%)	109 (4%)	22 (1%)	19	15

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	49	THR
1	H	84	PRO
1	P	84	PRO
1	S	84	PRO
1	T	84	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/123 (79%)	96 (99%)	1 (1%)	76	82
1	B	98/123 (80%)	94 (96%)	4 (4%)	30	31
1	C	97/123 (79%)	95 (98%)	2 (2%)	53	59
1	D	97/123 (79%)	94 (97%)	3 (3%)	40	43
1	E	97/123 (79%)	91 (94%)	6 (6%)	18	15
1	F	96/123 (78%)	94 (98%)	2 (2%)	53	59
1	G	97/123 (79%)	91 (94%)	6 (6%)	18	15
1	H	97/123 (79%)	94 (97%)	3 (3%)	40	43
1	I	97/123 (79%)	92 (95%)	5 (5%)	23	21
1	J	97/123 (79%)	96 (99%)	1 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	97/123 (79%)	93 (96%)	4 (4%)	30	31
1	L	97/123 (79%)	94 (97%)	3 (3%)	40	43
1	M	97/123 (79%)	92 (95%)	5 (5%)	23	21
1	N	97/123 (79%)	95 (98%)	2 (2%)	53	59
1	O	97/123 (79%)	97 (100%)	0	100	100
1	P	97/123 (79%)	91 (94%)	6 (6%)	18	15
1	Q	97/123 (79%)	93 (96%)	4 (4%)	30	31
1	R	97/123 (79%)	93 (96%)	4 (4%)	30	31
1	S	97/123 (79%)	91 (94%)	6 (6%)	18	15
1	T	97/123 (79%)	92 (95%)	5 (5%)	23	21
1	U	95/123 (77%)	91 (96%)	4 (4%)	30	30
1	V	95/123 (77%)	92 (97%)	3 (3%)	39	41
1	W	97/123 (79%)	94 (97%)	3 (3%)	40	43
1	X	97/123 (79%)	94 (97%)	3 (3%)	40	43
All	All	2324/2952 (79%)	2239 (96%)	85 (4%)	34	35

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	44	MET
1	T	124	LYS
1	R	101	THR
1	S	105	ASN
1	U	124	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	53	GLN
1	X	40	ASN
1	O	105	ASN
1	W	105	ASN
1	U	105	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	118/152 (77%)	0.07	2 (1%)	70	74	22, 28, 42, 54	0
1	B	119/152 (78%)	0.23	5 (4%)	36	42	21, 31, 44, 59	0
1	C	118/152 (77%)	0.22	4 (3%)	45	51	23, 31, 45, 59	0
1	D	118/152 (77%)	0.26	6 (5%)	28	33	21, 31, 47, 63	0
1	E	118/152 (77%)	0.25	4 (3%)	45	51	22, 31, 50, 61	0
1	F	117/152 (76%)	0.25	4 (3%)	45	51	24, 32, 46, 57	0
1	G	118/152 (77%)	0.28	6 (5%)	28	33	20, 29, 44, 59	0
1	H	118/152 (77%)	0.27	8 (6%)	17	21	23, 31, 47, 63	0
1	I	118/152 (77%)	0.14	4 (3%)	45	51	20, 27, 43, 52	0
1	J	118/152 (77%)	0.23	5 (4%)	36	42	22, 29, 44, 57	0
1	K	118/152 (77%)	0.21	3 (2%)	57	62	21, 31, 45, 62	0
1	L	118/152 (77%)	0.14	5 (4%)	36	42	20, 28, 41, 58	0
1	M	118/152 (77%)	0.22	4 (3%)	45	51	21, 29, 43, 60	0
1	N	118/152 (77%)	0.20	6 (5%)	28	33	25, 33, 46, 53	0
1	O	118/152 (77%)	0.36	7 (5%)	22	27	28, 37, 49, 62	0
1	P	118/152 (77%)	0.21	4 (3%)	45	51	23, 31, 44, 59	0
1	Q	118/152 (77%)	0.14	4 (3%)	45	51	18, 28, 42, 60	0
1	R	118/152 (77%)	0.09	3 (2%)	57	62	20, 28, 43, 62	0
1	S	118/152 (77%)	0.26	5 (4%)	36	42	24, 32, 45, 59	0
1	T	118/152 (77%)	0.29	7 (5%)	22	27	22, 31, 47, 58	0
1	U	116/152 (76%)	0.22	7 (6%)	21	27	19, 28, 47, 65	0
1	V	116/152 (76%)	0.44	8 (6%)	16	21	28, 34, 51, 61	0
1	W	118/152 (77%)	0.25	4 (3%)	45	51	22, 30, 45, 63	0
1	X	118/152 (77%)	0.27	8 (6%)	17	21	20, 28, 45, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2828/3648 (77%)	0.23	123 (4%)	35	41	18, 31, 46, 65	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	89	PHE	9.2
1	X	89	PHE	8.5
1	V	89	PHE	8.1
1	D	85	ASN	8.0
1	M	89	PHE	7.9

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	V	999	1/1	0.95	0.09	73,73,73,73	0
2	ZN	D	999	1/1	0.98	0.07	36,36,36,36	0
2	ZN	E	999	1/1	0.98	0.08	35,35,35,35	0
2	ZN	G	999	1/1	0.98	0.10	38,38,38,38	0
2	ZN	I	999	1/1	0.98	0.10	35,35,35,35	0
2	ZN	K	999	1/1	0.98	0.07	37,37,37,37	0
2	ZN	B	999	1/1	0.98	0.09	41,41,41,41	0
2	ZN	X	999	1/1	0.98	0.06	36,36,36,36	0
2	ZN	G	998	1/1	0.99	0.12	27,27,27,27	0
2	ZN	C	999	1/1	0.99	0.09	35,35,35,35	0
2	ZN	H	999	1/1	0.99	0.10	39,39,39,39	0
2	ZN	D	998	1/1	0.99	0.13	27,27,27,27	0
2	ZN	J	999	1/1	0.99	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	998	1/1	0.99	0.12	27,27,27,27	0
2	ZN	L	999	1/1	0.99	0.10	35,35,35,35	0
2	ZN	M	998	1/1	0.99	0.12	27,27,27,27	0
2	ZN	M	999	1/1	0.99	0.10	43,43,43,43	0
2	ZN	N	999	1/1	0.99	0.10	41,41,41,41	0
2	ZN	O	998	1/1	0.99	0.10	34,34,34,34	0
2	ZN	O	999	1/1	0.99	0.10	42,42,42,42	0
2	ZN	P	998	1/1	0.99	0.10	28,28,28,28	0
2	ZN	P	999	1/1	0.99	0.10	38,38,38,38	0
2	ZN	Q	999	1/1	0.99	0.07	37,37,37,37	0
2	ZN	R	999	1/1	0.99	0.09	34,34,34,34	0
2	ZN	T	999	1/1	0.99	0.10	43,43,43,43	0
2	ZN	U	999	1/1	0.99	0.10	33,33,33,33	0
2	ZN	V	998	1/1	0.99	0.09	29,29,29,29	0
2	ZN	A	999	1/1	0.99	0.07	36,36,36,36	0
2	ZN	F	999	1/1	0.99	0.09	38,38,38,38	0
2	ZN	E	998	1/1	1.00	0.11	27,27,27,27	0
2	ZN	K	998	1/1	1.00	0.11	29,29,29,29	0
2	ZN	C	998	1/1	1.00	0.12	27,27,27,27	0
2	ZN	Q	998	1/1	1.00	0.11	25,25,25,25	0
2	ZN	L	998	1/1	1.00	0.12	27,27,27,27	0
2	ZN	R	998	1/1	1.00	0.09	28,28,28,28	0
2	ZN	H	998	1/1	1.00	0.12	29,29,29,29	0
2	ZN	S	998	1/1	1.00	0.12	27,27,27,27	0
2	ZN	S	999	1/1	1.00	0.08	32,32,32,32	0
2	ZN	T	998	1/1	1.00	0.10	27,27,27,27	0
2	ZN	F	998	1/1	1.00	0.11	27,27,27,27	0
2	ZN	U	998	1/1	1.00	0.13	26,26,26,26	0
2	ZN	I	998	1/1	1.00	0.13	25,25,25,25	0
2	ZN	N	998	1/1	1.00	0.12	29,29,29,29	0
2	ZN	A	998	1/1	1.00	0.11	27,27,27,27	0
2	ZN	W	998	1/1	1.00	0.12	28,28,28,28	0
2	ZN	W	999	1/1	1.00	0.07	34,34,34,34	0
2	ZN	X	998	1/1	1.00	0.14	24,24,24,24	0
2	ZN	J	998	1/1	1.00	0.12	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.