wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 09:24 AM EDT

PDB ID	:	2X53
Title	:	Structure of the phage p2 baseplate in its activated conformation with Sr
Authors	:	Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; van Heel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on	:	2010-02-05
Resolution	:	3.90 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:

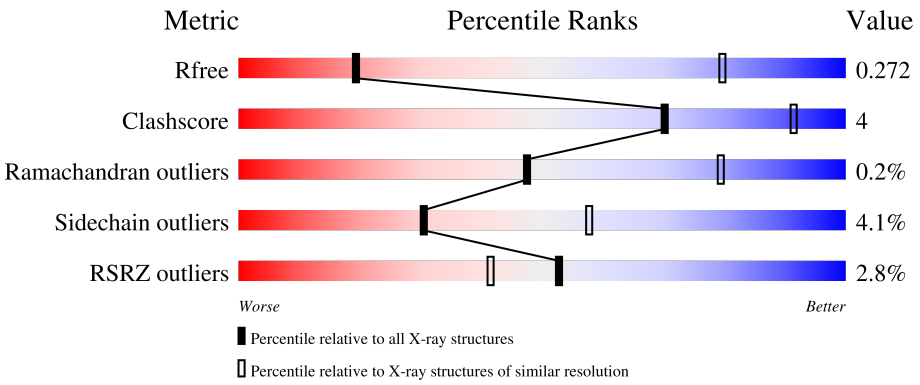
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	1	375	2% 85% 12% • •
1	Y	375	% 86% 12% • •
1	Z	375	% 85% 13% • •
2	A	263	90% 10%
2	B	263	92% 8%

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Mol	Chain	Length	Quality of chain
2	C	263	92% 8%
2	D	263	5% 90% 9%
2	E	263	5% 92% 8%
2	F	263	8% 92% 8%
2	G	263	9% 90% 10%
2	H	263	12% 93% 7%
2	I	263	8% 92% 8%
2	J	263	90% 10%
2	K	263	92% 8%
2	L	263	91% 9%
2	M	263	90% 10%
2	N	263	92% 8%
2	O	263	92% 8%
2	P	263	7% 92% 8%
2	Q	263	9% 91% 9%
2	R	263	10% 90% 10%
3	S	298	81% 16% •
3	T	298	79% 18% •
3	U	298	78% 20% •
3	V	298	81% 17% •
3	W	298	83% 14% •
3	X	298	% 81% 17% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 59742 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 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	372	3000	1918	493	581	8	0	0	0
1	Y	372	3000	1918	493	581	8	0	0	0
1	Z	372	3000	1918	493	581	8	0	0	0

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	263	2008	1260	346	396	6	0	0	0
2	B	263	2008	1260	346	396	6	0	0	0
2	C	263	2008	1260	346	396	6	0	0	0
2	D	263	2008	1260	346	396	6	0	0	0
2	E	263	2008	1260	346	396	6	0	0	0
2	F	263	2008	1260	346	396	6	0	0	0
2	G	263	2008	1260	346	396	6	0	0	0
2	H	263	2008	1260	346	396	6	0	0	0
2	I	263	2008	1260	346	396	6	0	0	0
2	J	263	2008	1260	346	396	6	0	0	0
2	K	263	2008	1260	346	396	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	263	2008	1260	346	396	6	0	0	0
2	M	263	2008	1260	346	396	6	0	0	0
2	N	263	2008	1260	346	396	6	0	0	0
2	O	263	2008	1260	346	396	6	0	0	0
2	P	263	2008	1260	346	396	6	0	0	0
2	Q	263	2008	1260	346	396	6	0	0	0
2	R	263	2008	1260	346	396	6	0	0	0

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S	298	2432	1565	392	469	6	0	0	0
3	T	298	2432	1565	392	469	6	0	0	0
3	U	298	2432	1565	392	469	6	0	0	0
3	V	298	2432	1565	392	469	6	0	0	0
3	W	298	2432	1565	392	469	6	0	0	0
3	X	298	2432	1565	392	469	6	0	0	0

- Molecule 4 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
4	S	1	1	1	0	0
4	T	1	1	1	0	0
4	U	1	1	1	0	0
4	V	1	1	1	0	0

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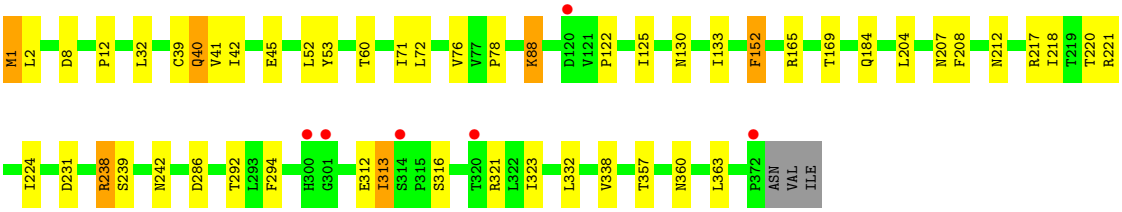
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
4	W	1	1	1	0	0
			Total	Sr		
4	X	1	1	1	0	0

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.

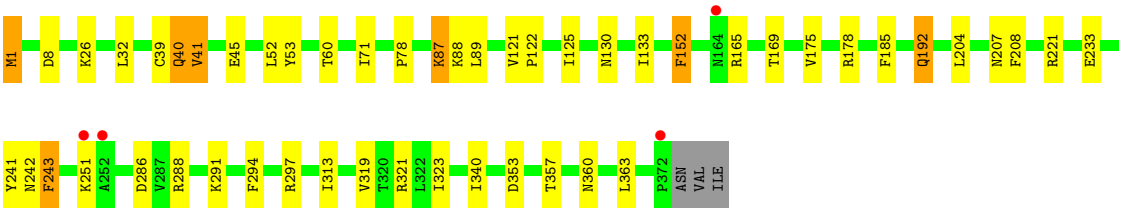
• Molecule 1: ORF16

Chain 1:



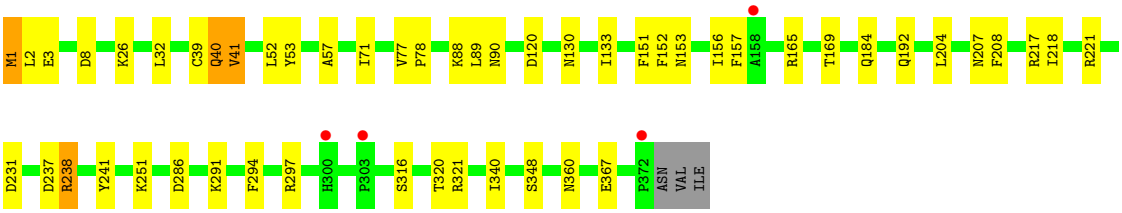
• Molecule 1: ORF16

Chain Y:



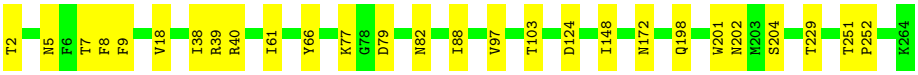
• Molecule 1: ORF16

Chain Z:



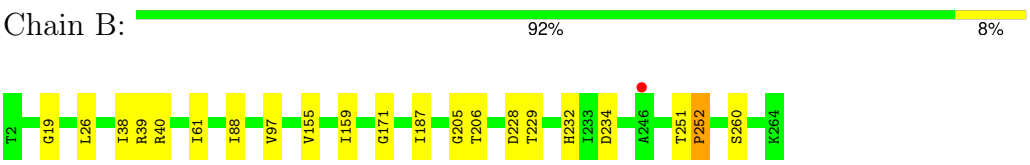
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain A:



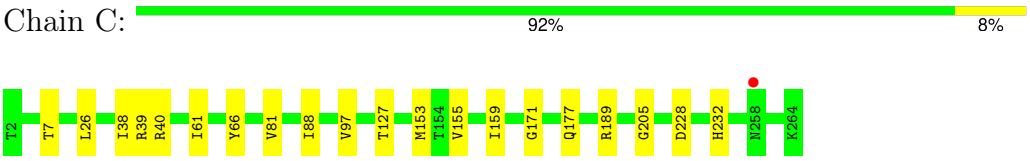
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain B:



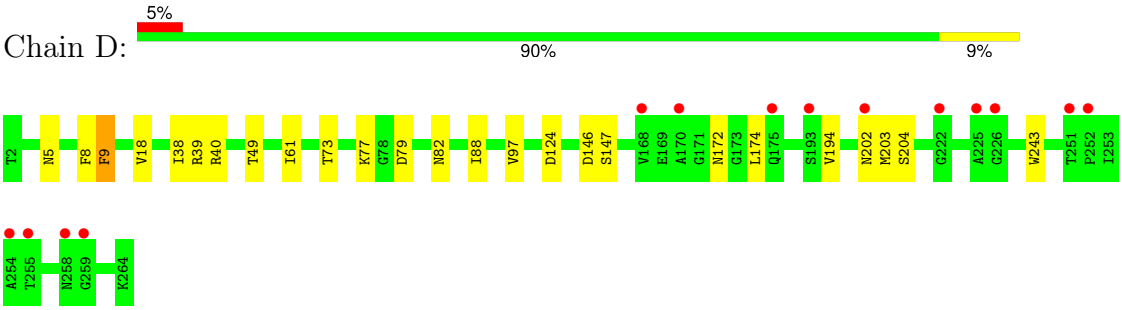
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain C:



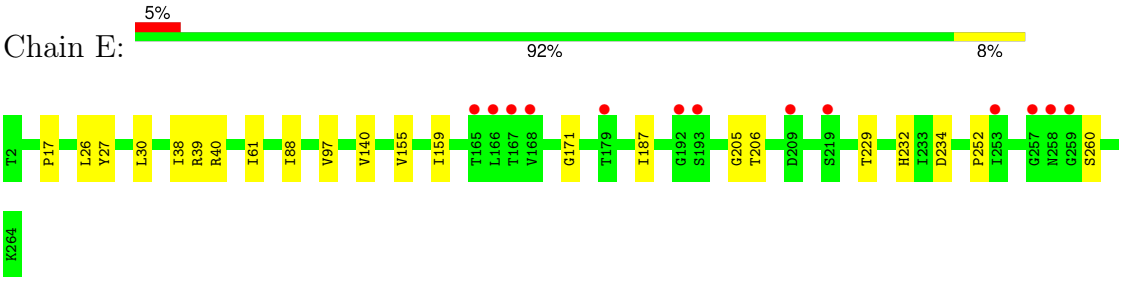
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain D:



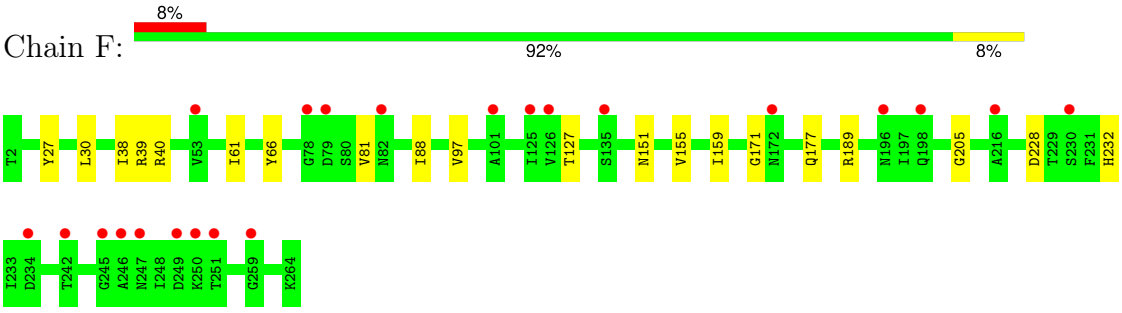
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain E:



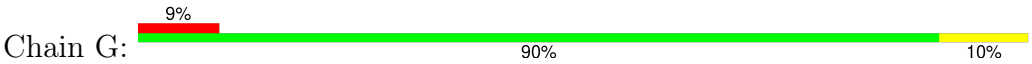
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

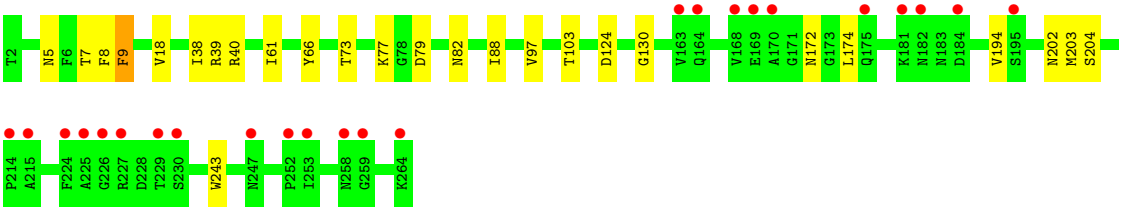
Chain F:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

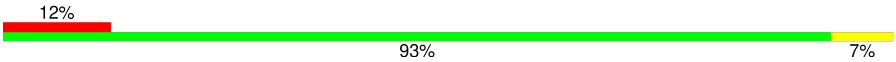
Chain G:

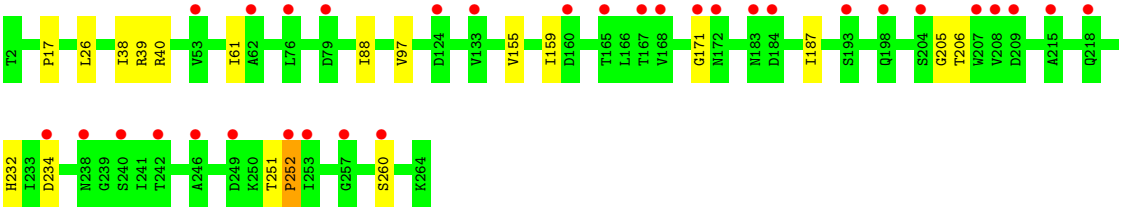




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

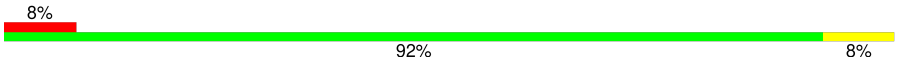
Chain H:

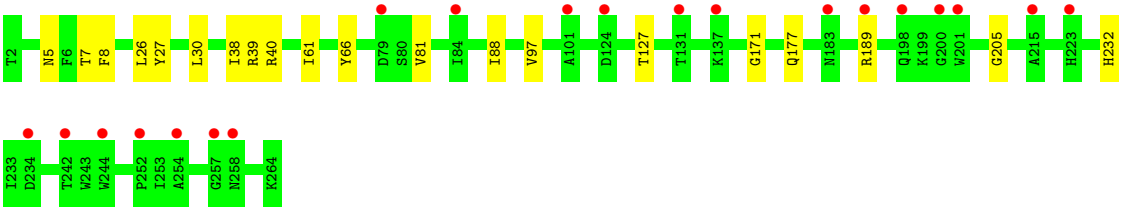




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

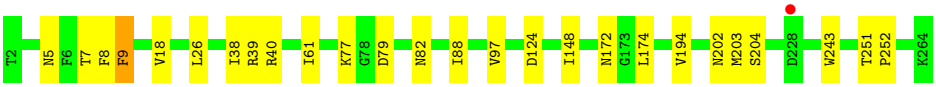
Chain I:





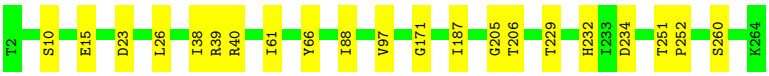
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain J:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain K:

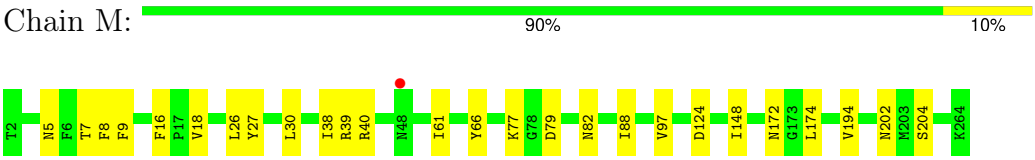


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain L:

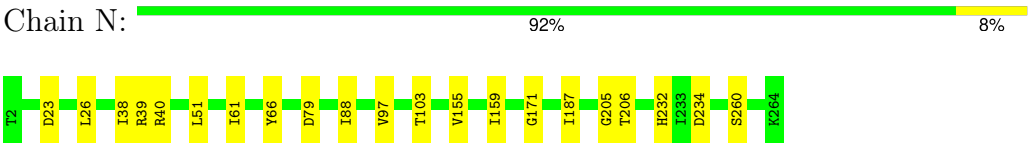
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain M:



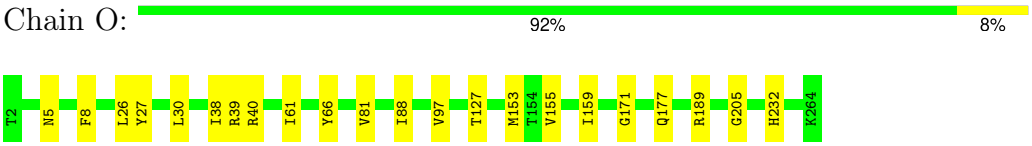
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain N:



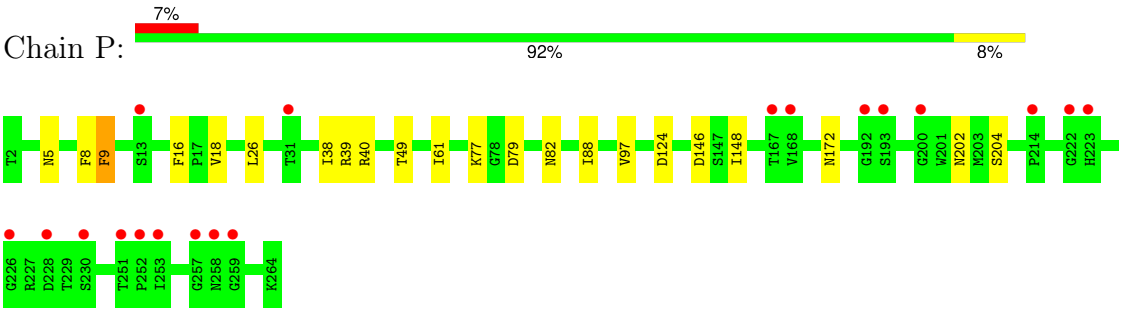
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain O:



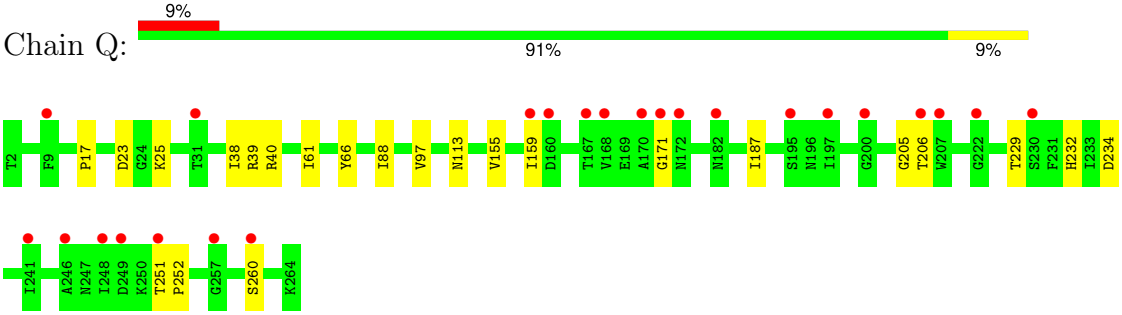
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain P:



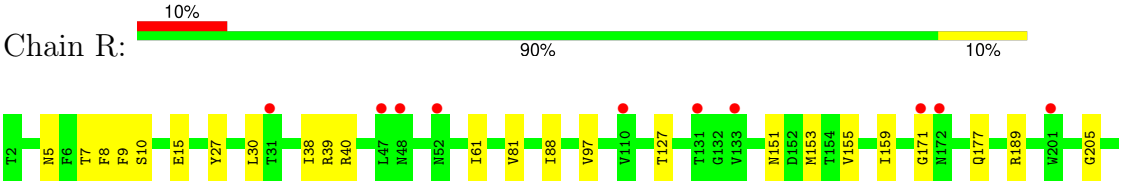
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

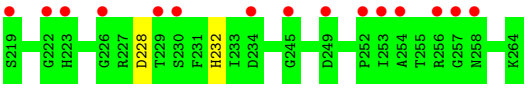
Chain Q:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

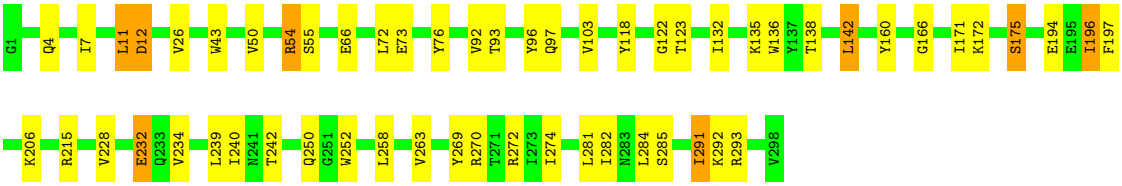
Chain R:





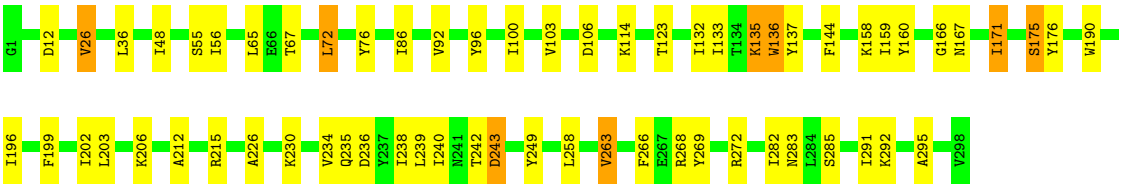
• Molecule 3: ORF15

Chain S:



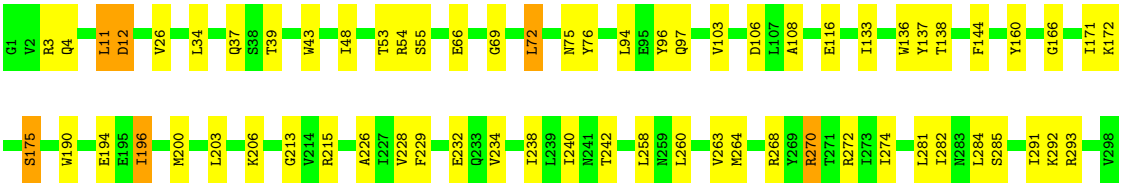
• Molecule 3: ORF15

Chain T:



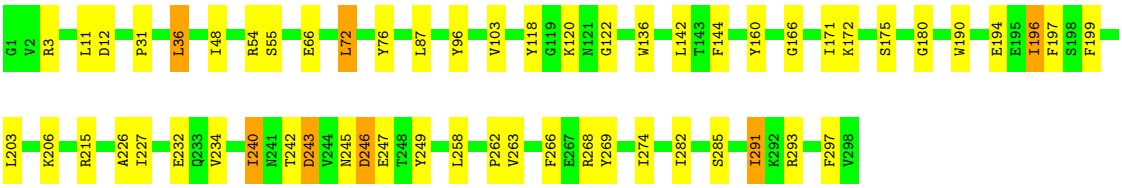
• Molecule 3: ORF15

Chain U:



• Molecule 3: ORF15

Chain V:

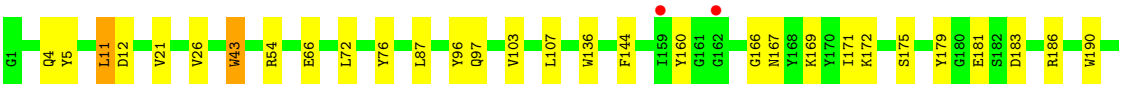


• Molecule 3: ORF15

Chain W:

• Molecule 3: ORF15

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	300.28Å 239.51Å 274.78Å 90.00° 124.36° 90.00°	Depositor
Resolution (Å)	39.31 – 3.90 39.15 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.31-3.90) 96.9 (39.15-3.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 3.87Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.229 , 0.242 0.260 , 0.272	Depositor DCC
R_{free} test set	4226 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 85.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	59742	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: SR

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	1	0.38	0/3069	0.64	0/4175
1	Y	0.38	0/3069	0.65	0/4175
1	Z	0.38	0/3069	0.63	0/4175
2	A	0.32	0/2048	0.63	0/2791
2	B	0.36	0/2048	0.58	0/2791
2	C	0.35	0/2048	0.59	0/2791
2	D	0.32	0/2048	0.61	0/2791
2	E	0.36	0/2048	0.58	0/2791
2	F	0.36	0/2048	0.58	0/2791
2	G	0.32	0/2048	0.62	0/2791
2	H	0.37	0/2048	0.58	0/2791
2	I	0.37	0/2048	0.58	0/2791
2	J	0.34	0/2048	0.63	0/2791
2	K	0.36	0/2048	0.59	0/2791
2	L	0.36	0/2048	0.58	0/2791
2	M	0.34	0/2048	0.63	0/2791
2	N	0.36	0/2048	0.58	0/2791
2	O	0.36	0/2048	0.58	0/2791
2	P	0.34	0/2048	0.63	0/2791
2	Q	0.37	0/2048	0.58	0/2791
2	R	0.37	0/2048	0.59	0/2791
3	S	0.36	0/2485	0.69	0/3356
3	T	0.36	0/2485	0.69	0/3356
3	U	0.35	0/2485	0.67	0/3356
3	V	0.36	0/2485	0.67	0/3356
3	W	0.35	0/2485	0.66	0/3356
3	X	0.36	0/2485	0.67	0/3356
All	All	0.36	0/60981	0.62	0/82899

There are no bond length outliers.

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	1	3000	0	2956	35	0
1	Y	3000	0	2956	25	0
1	Z	3000	0	2956	32	0
2	A	2008	0	1971	13	0
2	B	2008	0	1971	10	0
2	C	2008	0	1971	10	0
2	D	2008	0	1971	14	0
2	E	2008	0	1971	10	0
2	F	2008	0	1971	10	0
2	G	2008	0	1971	16	0
2	H	2008	0	1971	7	0
2	I	2008	0	1971	9	0
2	J	2008	0	1971	13	0
2	K	2008	0	1971	9	0
2	L	2008	0	1971	11	0
2	M	2008	0	1971	13	0
2	N	2008	0	1971	11	0
2	O	2008	0	1971	11	0
2	P	2008	0	1971	14	0
2	Q	2008	0	1971	10	0
2	R	2008	0	1971	16	0
3	S	2432	0	2394	34	0
3	T	2432	0	2394	35	0
3	U	2432	0	2394	35	0
3	V	2432	0	2394	28	0
3	W	2432	0	2394	23	0
3	X	2432	0	2394	40	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59742	0	58710	423	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 4.

The worst 5 of 423 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)
1:1:78:PRO:HG3	2:N:103:THR:HB	1.31	1.08
2:G:103:THR:HB	1:Z:78:PRO:HG3	1.41	1.00
3:S:242:THR:CG2	3:S:272:ARG:HG3	1.90	1.00
2:A:103:THR:HB	1:Y:78:PRO:HG3	1.48	0.94
1:1:42:ILE:HB	3:X:43:TRP:HZ2	1.33	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	1	370/375 (99%)	358 (97%)	12 (3%)	0	100	100
1	Y	370/375 (99%)	355 (96%)	15 (4%)	0	100	100
1	Z	370/375 (99%)	357 (96%)	13 (4%)	0	100	100
2	A	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	B	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	C	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	D	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	E	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	F	261/263 (99%)	246 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	H	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	I	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	J	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	K	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	L	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	M	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	N	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	O	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	P	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	Q	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	R	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
3	S	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	22	60
3	T	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	22	60
3	U	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	22	60
3	V	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	22	60
3	W	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	22	60
3	X	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	60
All	All	7584/7647 (99%)	7207 (95%)	365 (5%)	12 (0%)	47	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	175	SER
3	T	175	SER
3	U	175	SER
3	V	175	SER
3	W	175	SER

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	1	337/340 (99%)	324 (96%)	13 (4%)	32	59
1	Y	337/340 (99%)	319 (95%)	18 (5%)	22	52
1	Z	337/340 (99%)	321 (95%)	16 (5%)	26	55
2	A	227/227 (100%)	218 (96%)	9 (4%)	31	58
2	B	227/227 (100%)	221 (97%)	6 (3%)	46	68
2	C	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	D	227/227 (100%)	220 (97%)	7 (3%)	40	64
2	E	227/227 (100%)	221 (97%)	6 (3%)	46	68
2	F	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	G	227/227 (100%)	219 (96%)	8 (4%)	36	62
2	H	227/227 (100%)	220 (97%)	7 (3%)	40	64
2	I	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	J	227/227 (100%)	219 (96%)	8 (4%)	36	62
2	K	227/227 (100%)	221 (97%)	6 (3%)	46	68
2	L	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	M	227/227 (100%)	219 (96%)	8 (4%)	36	62
2	N	227/227 (100%)	221 (97%)	6 (3%)	46	68
2	O	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	P	227/227 (100%)	220 (97%)	7 (3%)	40	64
2	Q	227/227 (100%)	220 (97%)	7 (3%)	40	64
2	R	227/227 (100%)	223 (98%)	4 (2%)	59	77
3	S	264/264 (100%)	246 (93%)	18 (7%)	16	45
3	T	264/264 (100%)	247 (94%)	17 (6%)	17	47
3	U	264/264 (100%)	241 (91%)	23 (9%)	10	37
3	V	264/264 (100%)	241 (91%)	23 (9%)	10	37
3	W	264/264 (100%)	244 (92%)	20 (8%)	13	42
3	X	264/264 (100%)	247 (94%)	17 (6%)	17	47
All	All	6681/6690 (100%)	6409 (96%)	272 (4%)	30	58

5 of 272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	X	228	VAL
1	Y	1	MET
1	Z	39	CYS
2	N	232	HIS
2	N	38	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
3	T	102	GLN
1	Y	143	ASN
3	T	235	GLN
3	V	250	GLN
2	G	172	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 6 ligands modelled in this entry, 6 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	1	372/375 (99%)	0.16	6 (1%)	72	62	63, 97, 170, 239	0
1	Y	372/375 (99%)	0.04	4 (1%)	80	73	62, 94, 151, 270	0
1	Z	372/375 (99%)	0.12	4 (1%)	80	73	63, 98, 166, 246	0
2	A	263/263 (100%)	-0.16	0	100	100	44, 76, 105, 140	0
2	B	263/263 (100%)	-0.03	1 (0%)	92	87	55, 88, 126, 147	0
2	C	263/263 (100%)	0.02	1 (0%)	92	87	55, 90, 137, 172	0
2	D	263/263 (100%)	0.24	14 (5%)	26	22	52, 106, 248, 290	0
2	E	263/263 (100%)	0.41	13 (4%)	29	24	64, 121, 259, 286	0
2	F	263/263 (100%)	0.49	22 (8%)	11	9	57, 144, 245, 291	0
2	G	263/263 (100%)	0.37	24 (9%)	9	7	60, 126, 249, 285	0
2	H	263/263 (100%)	0.77	32 (12%)	4	4	97, 155, 233, 282	0
2	I	263/263 (100%)	0.68	20 (7%)	13	10	75, 156, 262, 297	0
2	J	263/263 (100%)	0.04	1 (0%)	92	87	55, 102, 163, 246	0
2	K	263/263 (100%)	0.03	0	100	100	52, 84, 175, 233	0
2	L	263/263 (100%)	0.08	1 (0%)	92	87	62, 102, 162, 220	0
2	M	263/263 (100%)	0.18	1 (0%)	92	87	76, 126, 166, 208	0
2	N	263/263 (100%)	0.03	0	100	100	60, 95, 142, 163	0
2	O	263/263 (100%)	0.23	0	100	100	85, 128, 168, 184	0
2	P	263/263 (100%)	0.45	19 (7%)	15	11	65, 132, 296, 298	0
2	Q	263/263 (100%)	0.71	24 (9%)	9	7	96, 154, 288, 292	0
2	R	263/263 (100%)	0.72	25 (9%)	8	6	83, 160, 292, 300	0
3	S	298/298 (100%)	-0.28	0	100	100	41, 64, 106, 124	0
3	T	298/298 (100%)	-0.32	0	100	100	42, 65, 113, 145	0
3	U	298/298 (100%)	-0.23	0	100	100	43, 71, 129, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	V	298/298 (100%)	-0.25	0 100 100	44, 66, 101, 127	0
3	W	298/298 (100%)	-0.21	1 (0%) 94 90	40, 67, 132, 161	0
3	X	298/298 (100%)	-0.20	2 (0%) 87 82	40, 67, 158, 202	0
All	All	7638/7647 (99%)	0.14	215 (2%) 53 41	40, 98, 207, 300	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	226	GLY	5.6
2	R	252	PRO	5.3
2	I	258	ASN	4.8
2	D	254	ALA	4.6
1	Y	372	PRO	4.2

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
4	SR	U	1299	1/1	0.93	0.26	82,82,82,82	0
4	SR	S	1299	1/1	0.94	0.25	87,87,87,87	0
4	SR	V	1299	1/1	0.96	0.26	80,80,80,80	0
4	SR	X	1299	1/1	0.97	0.25	83,83,83,83	0
4	SR	W	1299	1/1	0.98	0.29	80,80,80,80	0
4	SR	T	1299	1/1	0.98	0.27	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.