wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:43 AM GMT

PDB ID	:	3MUU
Title	:	Crystal structure of the Sindbis virus E2-E1 heterodimer at low pH
Authors	:	Li, L.; Jose, J.; Xiang, Y.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2010-05-03
Resolution	:	3.29 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

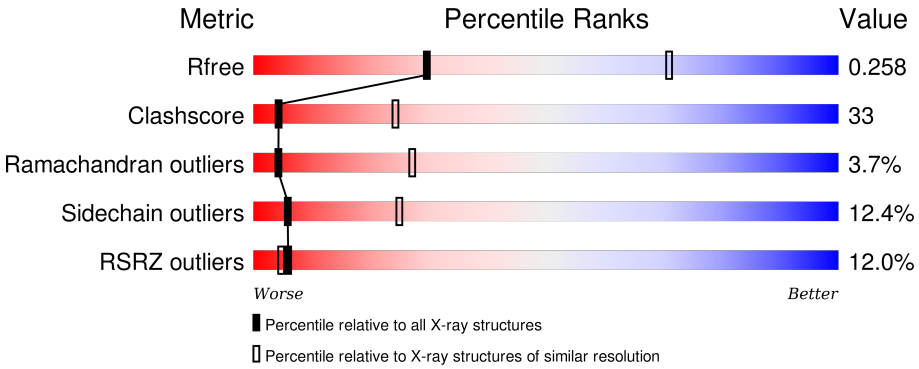
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.29 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	750	9% 39% 36% 7% 17%
1	B	750	9% 37% 38% 7% 17%
1	C	750	9% 38% 37% 7% 17%
1	D	750	11% 39% 36% 8% 17%
1	E	750	10% 40% 35% 7% 17%

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Mol	Chain	Length	Quality of chain
1	F	750	10% 39% 36% 7% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	751	X	-	-	-
2	MAN	B	754	-	-	-	X
2	MAN	E	754	-	-	-	X
2	NAG	F	751	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29159 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 Structural polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	Se	0	0	0
			4767	3015	808	910	24	10			
1	B	622	Total	C	N	O	S	Se	0	0	0
			4761	3013	808	906	24	10			
1	C	622	Total	C	N	O	S	Se	0	0	0
			4761	3012	807	908	24	10			
1	D	622	Total	C	N	O	S	Se	0	0	0
			4760	3009	807	910	24	10			
1	E	623	Total	C	N	O	S	Se	0	0	0
			4761	3012	808	907	24	10			
1	F	618	Total	C	N	O	S	Se	0	0	0
			4727	2990	801	902	24	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	GLY	-	LINKER	UNP P03316
A	346	GLY	-	LINKER	UNP P03316
A	347	GLY	-	LINKER	UNP P03316
A	348	SER	-	LINKER	UNP P03316
A	349	TRP	-	LINKER	UNP P03316
A	350	SER	-	LINKER	UNP P03316
A	351	HIS	-	LINKER	UNP P03316
A	352	PRO	-	LINKER	UNP P03316
A	353	GLN	-	LINKER	UNP P03316
A	354	PHE	-	LINKER	UNP P03316
A	355	GLU	-	LINKER	UNP P03316
A	356	LYS	-	LINKER	UNP P03316
A	357	GLY	-	LINKER	UNP P03316
A	358	GLY	-	LINKER	UNP P03316
A	359	GLY	-	LINKER	UNP P03316
A	360	GLY	-	LINKER	UNP P03316
A	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	GLY	-	LINKER	UNP P03316
B	346	GLY	-	LINKER	UNP P03316
B	347	GLY	-	LINKER	UNP P03316
B	348	SER	-	LINKER	UNP P03316
B	349	TRP	-	LINKER	UNP P03316
B	350	SER	-	LINKER	UNP P03316
B	351	HIS	-	LINKER	UNP P03316
B	352	PRO	-	LINKER	UNP P03316
B	353	GLN	-	LINKER	UNP P03316
B	354	PHE	-	LINKER	UNP P03316
B	355	GLU	-	LINKER	UNP P03316
B	356	LYS	-	LINKER	UNP P03316
B	357	GLY	-	LINKER	UNP P03316
B	358	GLY	-	LINKER	UNP P03316
B	359	GLY	-	LINKER	UNP P03316
B	360	GLY	-	LINKER	UNP P03316
B	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
C	345	GLY	-	LINKER	UNP P03316
C	346	GLY	-	LINKER	UNP P03316
C	347	GLY	-	LINKER	UNP P03316
C	348	SER	-	LINKER	UNP P03316
C	349	TRP	-	LINKER	UNP P03316
C	350	SER	-	LINKER	UNP P03316
C	351	HIS	-	LINKER	UNP P03316
C	352	PRO	-	LINKER	UNP P03316
C	353	GLN	-	LINKER	UNP P03316
C	354	PHE	-	LINKER	UNP P03316
C	355	GLU	-	LINKER	UNP P03316
C	356	LYS	-	LINKER	UNP P03316
C	357	GLY	-	LINKER	UNP P03316
C	358	GLY	-	LINKER	UNP P03316
C	359	GLY	-	LINKER	UNP P03316
C	360	GLY	-	LINKER	UNP P03316
C	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
D	345	GLY	-	LINKER	UNP P03316
D	346	GLY	-	LINKER	UNP P03316
D	347	GLY	-	LINKER	UNP P03316
D	348	SER	-	LINKER	UNP P03316
D	349	TRP	-	LINKER	UNP P03316
D	350	SER	-	LINKER	UNP P03316
D	351	HIS	-	LINKER	UNP P03316
D	352	PRO	-	LINKER	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
D	353	GLN	-	LINKER	UNP P03316
D	354	PHE	-	LINKER	UNP P03316
D	355	GLU	-	LINKER	UNP P03316
D	356	LYS	-	LINKER	UNP P03316
D	357	GLY	-	LINKER	UNP P03316
D	358	GLY	-	LINKER	UNP P03316
D	359	GLY	-	LINKER	UNP P03316
D	360	GLY	-	LINKER	UNP P03316
D	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
E	345	GLY	-	LINKER	UNP P03316
E	346	GLY	-	LINKER	UNP P03316
E	347	GLY	-	LINKER	UNP P03316
E	348	SER	-	LINKER	UNP P03316
E	349	TRP	-	LINKER	UNP P03316
E	350	SER	-	LINKER	UNP P03316
E	351	HIS	-	LINKER	UNP P03316
E	352	PRO	-	LINKER	UNP P03316
E	353	GLN	-	LINKER	UNP P03316
E	354	PHE	-	LINKER	UNP P03316
E	355	GLU	-	LINKER	UNP P03316
E	356	LYS	-	LINKER	UNP P03316
E	357	GLY	-	LINKER	UNP P03316
E	358	GLY	-	LINKER	UNP P03316
E	359	GLY	-	LINKER	UNP P03316
E	360	GLY	-	LINKER	UNP P03316
E	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316
F	345	GLY	-	LINKER	UNP P03316
F	346	GLY	-	LINKER	UNP P03316
F	347	GLY	-	LINKER	UNP P03316
F	348	SER	-	LINKER	UNP P03316
F	349	TRP	-	LINKER	UNP P03316
F	350	SER	-	LINKER	UNP P03316
F	351	HIS	-	LINKER	UNP P03316
F	352	PRO	-	LINKER	UNP P03316
F	353	GLN	-	LINKER	UNP P03316
F	354	PHE	-	LINKER	UNP P03316
F	355	GLU	-	LINKER	UNP P03316
F	356	LYS	-	LINKER	UNP P03316
F	357	GLY	-	LINKER	UNP P03316
F	358	GLY	-	LINKER	UNP P03316
F	359	GLY	-	LINKER	UNP P03316
F	360	GLY	-	LINKER	UNP P03316

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Chain	Residue	Modelled	Actual	Comment	Reference
F	435	GLY	ASP	ENGINEERED MUTATION	UNP P03316

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		
2	B	4	Total	C	N	O	0	0
			50	28	2	20		
2	B	4	Total	C	N	O	0	0
			50	28	2	20		
2	C	4	Total	C	N	O	0	0
			50	28	2	20		
2	C	4	Total	C	N	O	0	0
			50	28	2	20		
2	D	4	Total	C	N	O	0	0
			50	28	2	20		
2	E	4	Total	C	N	O	0	0
			50	28	2	20		
2	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	E	5	Total	C	N	O	0	0
			61	34	2	25		
3	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

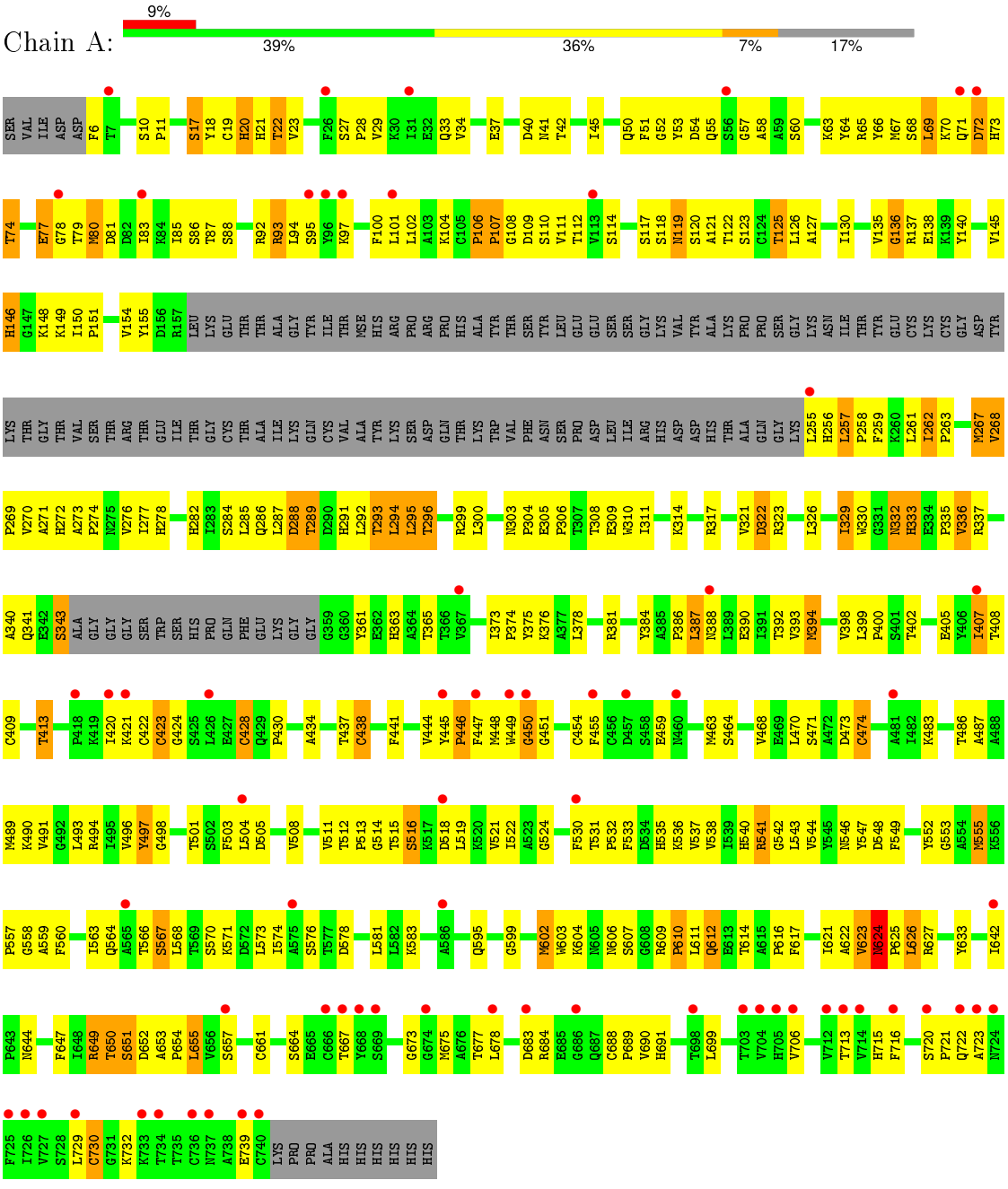
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

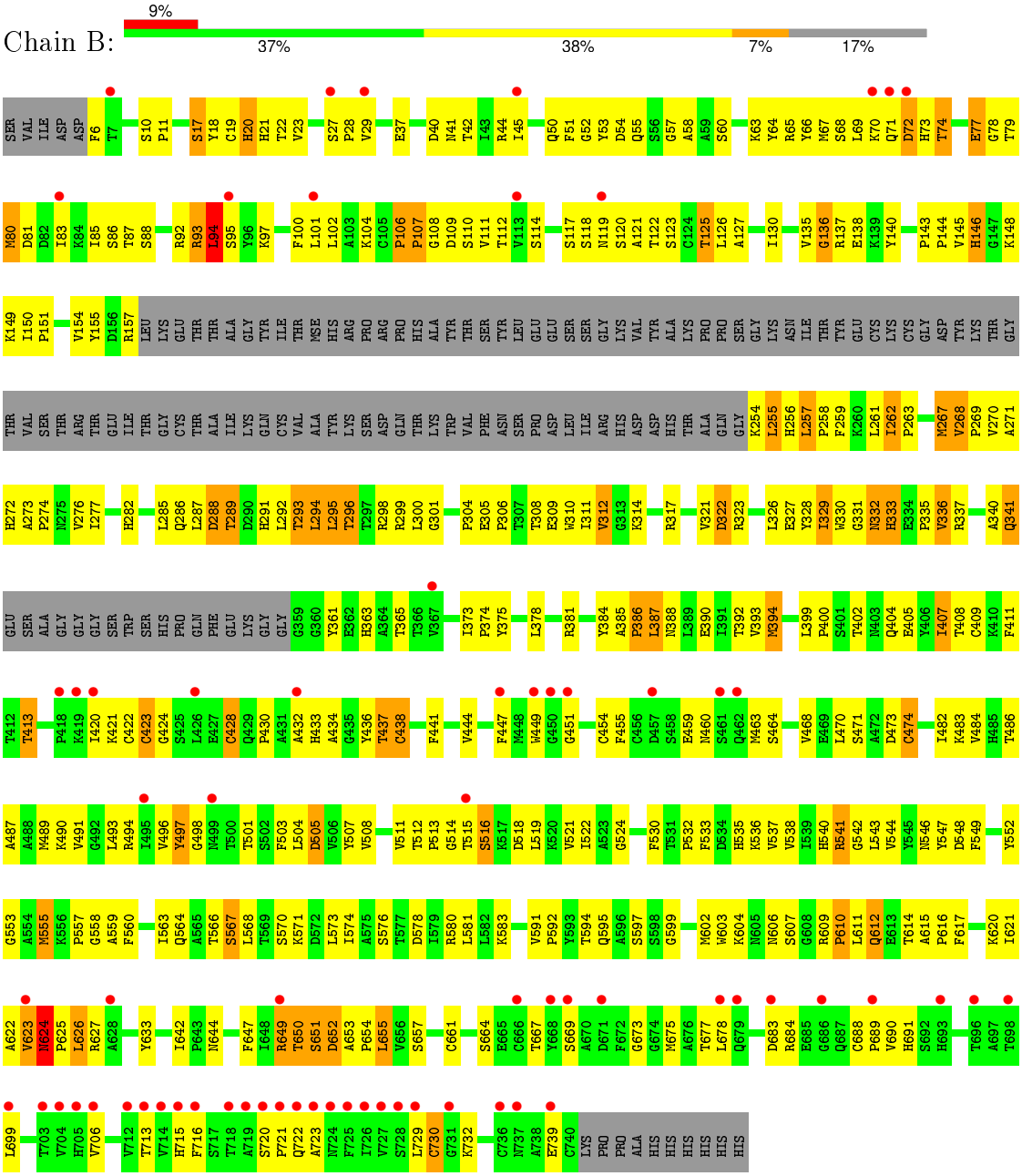
- Molecule 1: Structural polyprotein

Chain A:



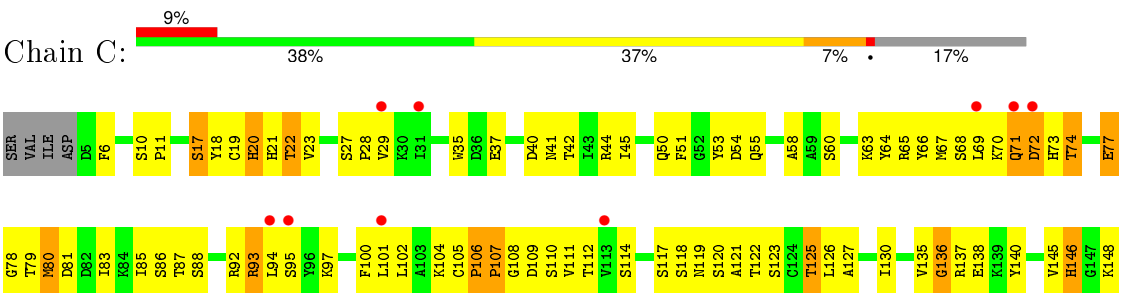
- Molecule 1: Structural polyprotein

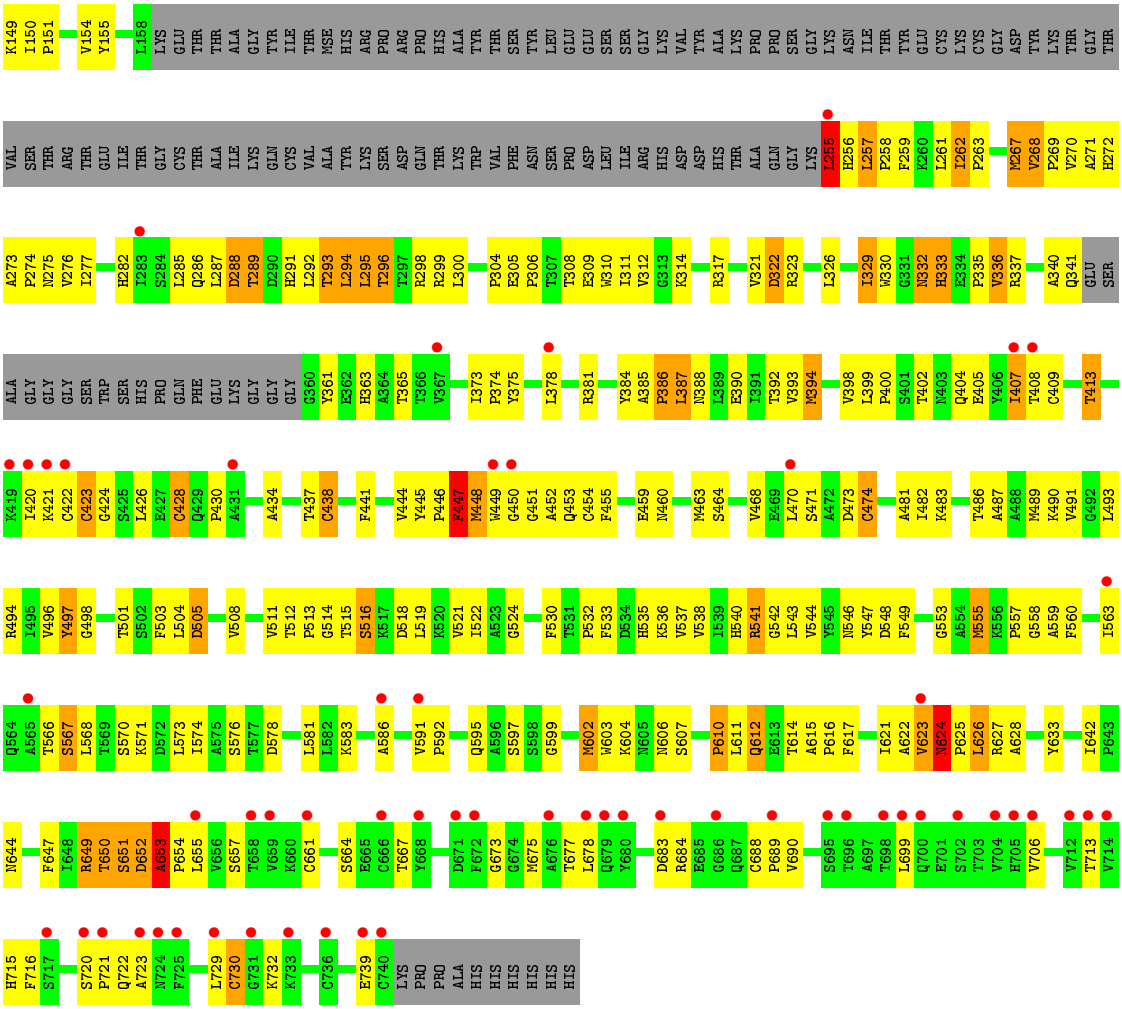
Chain B:



- Molecule 1: Structural polyprotein

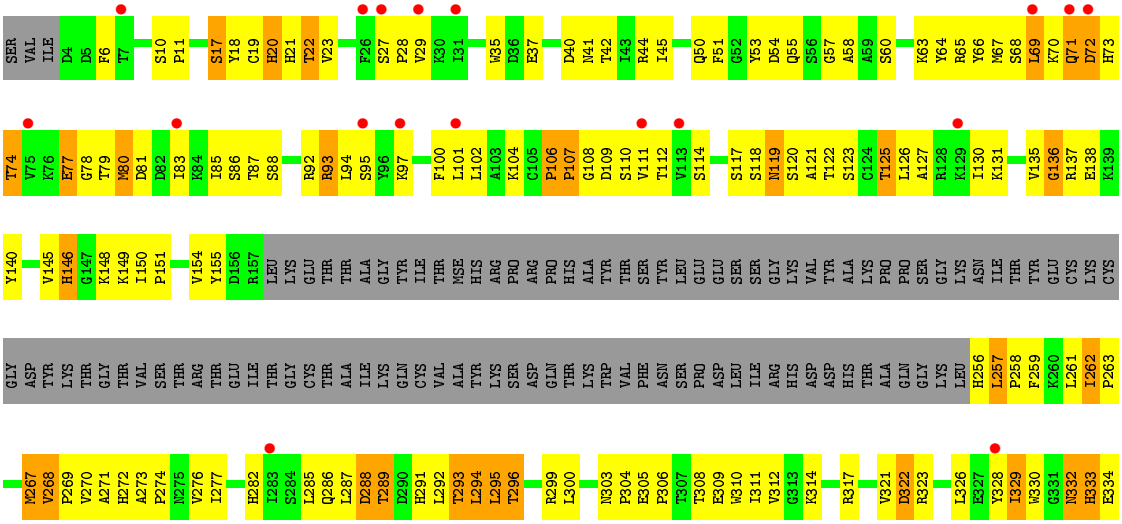
Chain C:

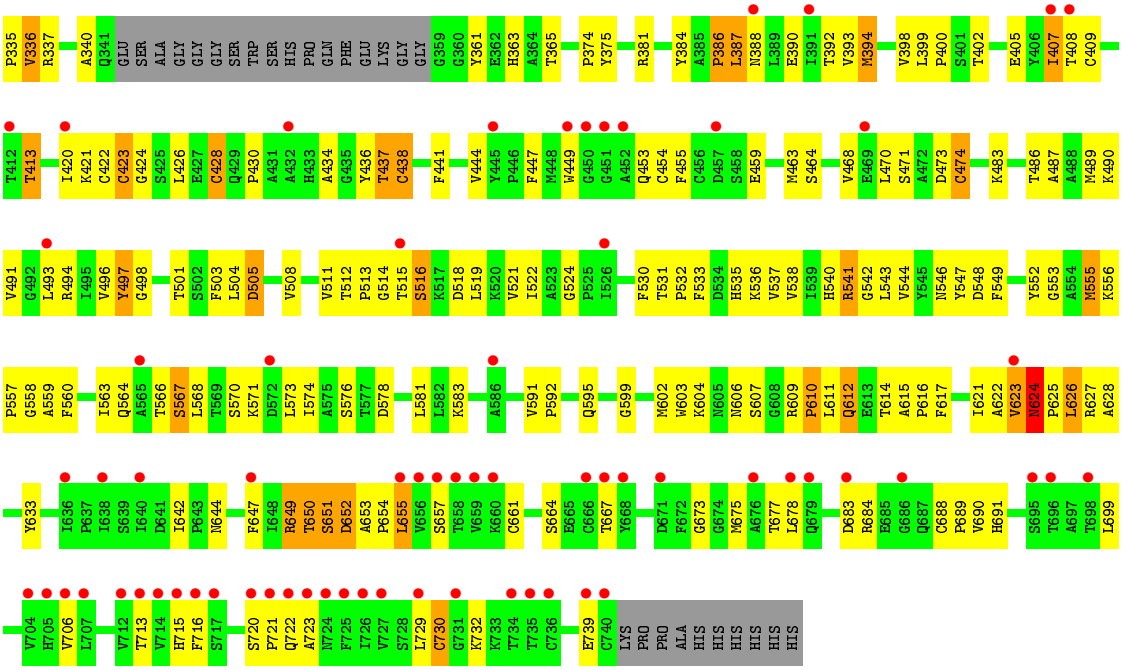




• Molecule 1: Structural polyprotein

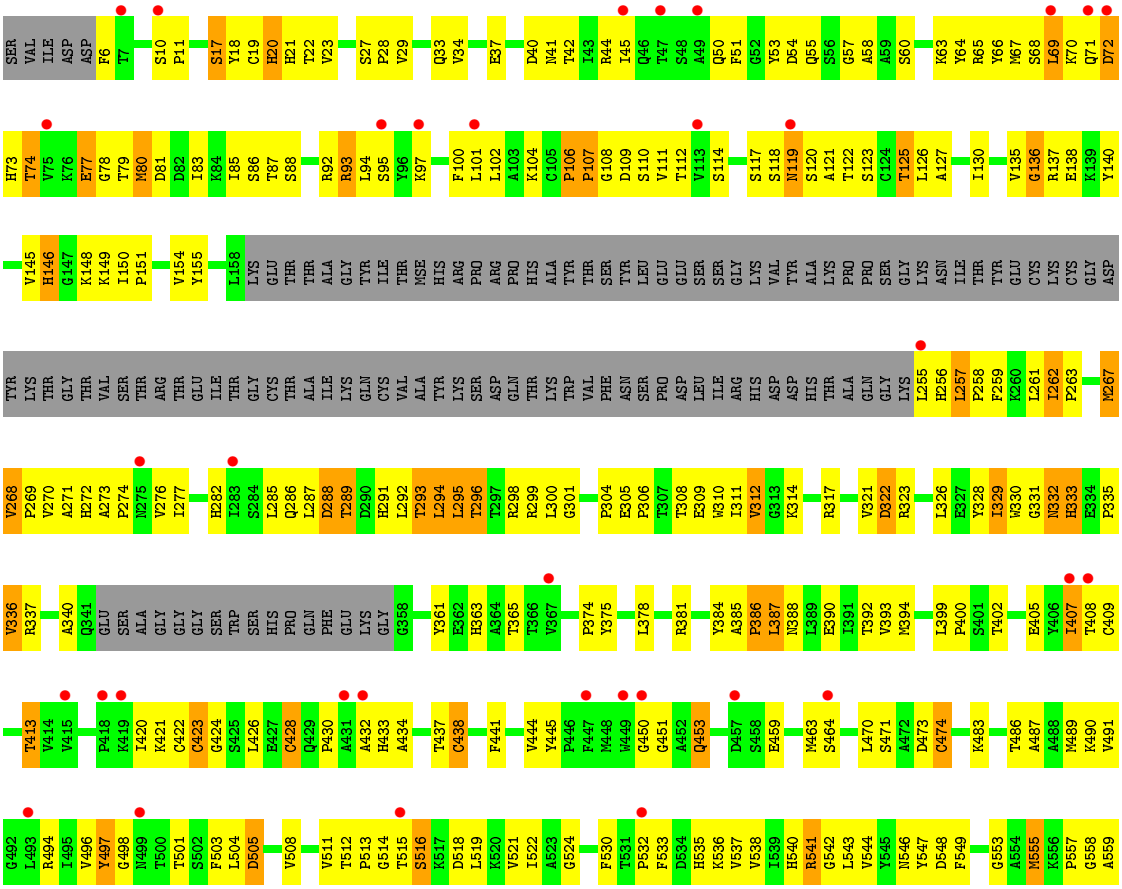
Chain D:

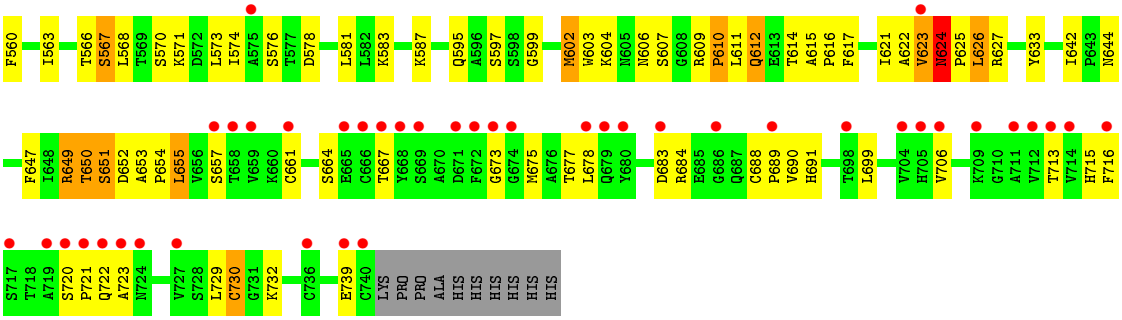


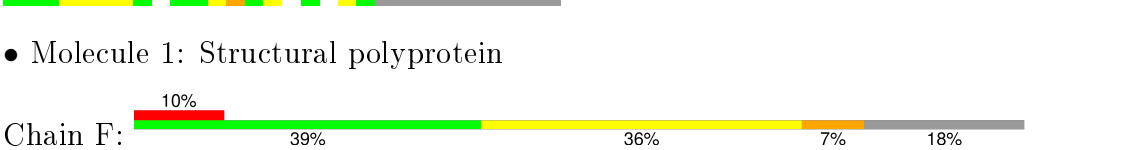


• Molecule 1: Structural polyprotein

Chain E:

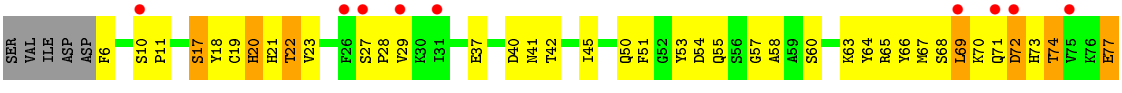


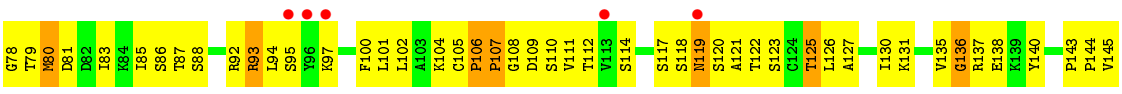


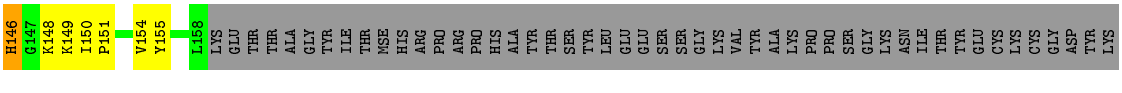


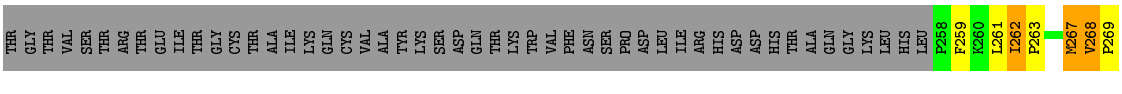
• Molecule 1: Structural polyprotein

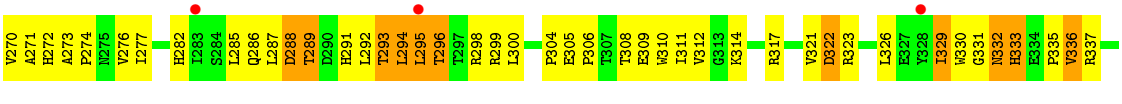
Chain F:

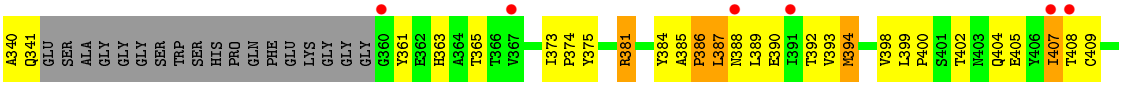


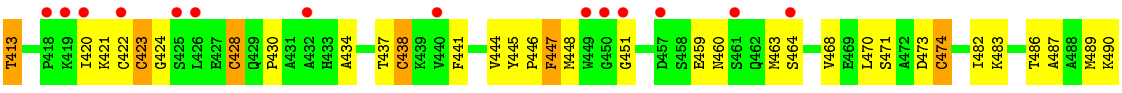


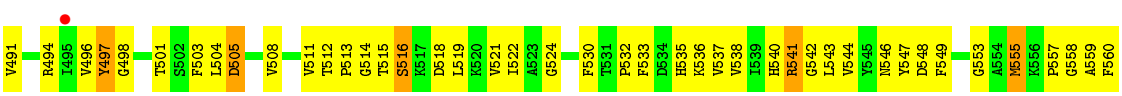


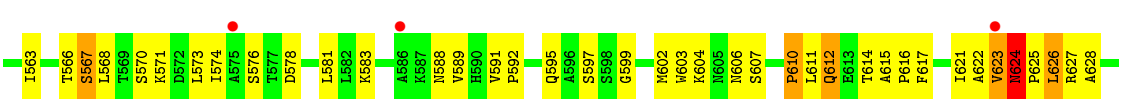


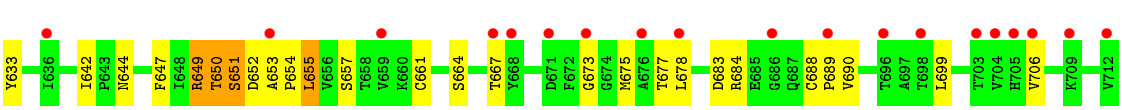












4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.48Å 158.43Å 160.68Å 60.42° 89.80° 89.65°	Depositor
Resolution (Å)	60.72 – 3.29 60.72 – 3.29	Depositor EDS
% Data completeness (in resolution range)	92.4 (60.72-3.29) 77.1 (60.72-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.26Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, R_{free}	0.239 , 0.252 0.246 , 0.258	Depositor DCC
R_{free} test set	4173 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	87.2	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 97.3	EDS
Estimated twinning fraction	0.033 for h,k-l,k 0.033 for h,l,-k+l 0.297 for h,-l,k-l 0.297 for h,-k+l,-k 0.037 for h,-k,-l 0.408 for -h,k,k-l 0.289 for -h,-l,-k 0.033 for -h,k-l,-l 0.309 for -h,-k+l,l 0.039 for -h,-k,-k+l 0.033 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 82963 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29159	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.35	0/4876	0.58	0/6624
1	B	0.35	0/4870	0.60	1/6615 (0.0%)
1	C	0.38	1/4870 (0.0%)	0.60	1/6617 (0.0%)
1	D	0.35	0/4869	0.58	0/6615
1	E	0.35	0/4870	0.58	0/6616
1	F	0.36	0/4835	0.67	3/6568 (0.0%)
All	All	0.36	1/29190 (0.0%)	0.60	5/39655 (0.0%)

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	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
2	A	1	0
2	F	1	0
All	All	2	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	653	ALA	C-N	7.00	1.47	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	381	ARG	NE-CZ-NH1	-19.90	110.35	120.30
1	F	381	ARG	NE-CZ-NH2	17.34	128.97	120.30
1	B	94	LEU	CA-CB-CG	-7.54	97.95	115.30
1	F	381	ARG	CD-NE-CZ	7.40	133.97	123.60
1	C	255	LEU	CB-CG-CD2	5.25	119.92	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	751	NAG	C1
2	F	751	NAG	C1

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	VAL	Peptide
1	A	624	ASN	Peptide
1	B	254	LYS	Peptide
1	B	623	VAL	Peptide
1	B	624	ASN	Peptide

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	4767	0	4659	316	0
1	B	4761	0	4661	335	0
1	C	4761	0	4651	329	0
1	D	4760	0	4645	320	0
1	E	4761	0	4653	311	0
1	F	4727	0	4619	304	0
2	A	50	0	42	2	0
2	B	100	0	86	2	0
2	C	100	0	85	4	0
2	D	50	0	42	1	0
2	E	50	0	42	0	0
2	F	50	0	43	0	0
3	A	61	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	61	0	52	2	0
3	F	61	0	52	6	0
4	D	39	0	34	2	0
All	All	29159	0	28418	1903	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 33.

The worst 5 of 1903 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:D:22:THR:HG21	1:E:104:LYS:HD2	1.29	1.14
1:D:88:SER:HB3	1:D:107:PRO:HG3	1.10	1.09
1:B:507:TYR:CE1	1:D:625:PRO:HG2	1.88	1.09
1:B:255:LEU:HG	1:B:256:HIS:H	1.14	1.08
1:B:88:SER:HB3	1:B:107:PRO:HG3	1.09	1.08

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	617/750 (82%)	501 (81%)	92 (15%)	24 (4%)	4 25
1	B	616/750 (82%)	499 (81%)	96 (16%)	21 (3%)	5 29
1	C	616/750 (82%)	500 (81%)	92 (15%)	24 (4%)	4 25
1	D	616/750 (82%)	502 (82%)	92 (15%)	22 (4%)	4 28
1	E	617/750 (82%)	505 (82%)	90 (15%)	22 (4%)	4 28
1	F	612/750 (82%)	503 (82%)	87 (14%)	22 (4%)	4 28
All	All	3694/4500 (82%)	3010 (82%)	549 (15%)	135 (4%)	4 27

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	117	SER
1	A	434	ALA
1	A	650	THR
1	A	730	CYS

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	534/630 (85%)	468 (88%)	66 (12%)	6	25
1	B	533/630 (85%)	466 (87%)	67 (13%)	5	24
1	C	533/630 (85%)	466 (87%)	67 (13%)	5	24
1	D	533/630 (85%)	469 (88%)	64 (12%)	6	27
1	E	532/630 (84%)	466 (88%)	66 (12%)	6	25
1	F	529/630 (84%)	464 (88%)	65 (12%)	6	25
All	All	3194/3780 (84%)	2799 (88%)	395 (12%)	6	25

5 of 395 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	474	CYS
1	D	289	THR
1	F	405	GLU
1	C	518	ASP
1	D	17	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	546	ASN
1	D	291	HIS

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Mol	Chain	Res	Type
1	F	333	HIS
1	C	595	GLN
1	D	46	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

50 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	751	1,2	14,14,15	0.39	0	15,19,21	2.19	1 (6%)
2	NAG	A	752	2	14,14,15	0.52	0	15,19,21	2.01	2 (13%)
2	BMA	A	753	2	11,11,12	1.75	3 (27%)	14,15,17	4.36	12 (85%)
2	MAN	A	754	2	11,11,12	0.87	1 (9%)	14,15,17	2.39	4 (28%)
3	NAG	A	761	1,3	14,14,15	0.67	0	15,19,21	1.37	2 (13%)
3	NAG	A	762	3	14,14,15	0.46	0	15,19,21	1.22	1 (6%)
3	BMA	A	763	3	11,11,12	2.15	4 (36%)	14,15,17	3.27	9 (64%)
3	MAN	A	764	3	11,11,12	0.41	0	14,15,17	1.65	2 (14%)
3	MAN	A	765	3	11,11,12	0.49	0	14,15,17	1.52	1 (7%)
2	NAG	B	751	1,2	14,14,15	0.73	0	15,19,21	0.99	0
2	NAG	B	752	2	14,14,15	0.81	0	15,19,21	1.67	2 (13%)
2	BMA	B	753	2	11,11,12	2.25	5 (45%)	14,15,17	3.10	9 (64%)
2	MAN	B	754	2	11,11,12	0.52	0	14,15,17	1.17	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	761	1,2	14,14,15	0.53	0	15,19,21	1.20	1 (6%)
2	NAG	B	762	2	14,14,15	0.57	0	15,19,21	1.50	3 (20%)
2	BMA	B	763	2	11,11,12	1.85	4 (36%)	14,15,17	3.79	9 (64%)
2	MAN	B	764	2	11,11,12	0.59	0	14,15,17	0.77	0
2	NAG	C	751	1,2	14,14,15	0.66	0	15,19,21	0.78	0
2	NAG	C	752	2	14,14,15	0.61	0	15,19,21	0.81	1 (6%)
2	BMA	C	753	2	11,11,12	2.13	4 (36%)	14,15,17	3.82	9 (64%)
2	MAN	C	754	2	11,11,12	0.77	1 (9%)	14,15,17	1.81	5 (35%)
2	NAG	C	761	1,2	14,14,15	0.44	0	15,19,21	2.02	2 (13%)
2	NAG	C	762	2	14,14,15	0.47	0	15,19,21	3.08	4 (26%)
2	BMA	C	763	2	11,11,12	1.85	3 (27%)	14,15,17	3.48	9 (64%)
2	MAN	C	764	2	11,11,12	0.44	0	14,15,17	1.90	2 (14%)
2	NAG	D	751	1,2	14,14,15	0.74	0	15,19,21	2.30	5 (33%)
2	NAG	D	752	2	14,14,15	0.56	0	15,19,21	1.65	3 (20%)
2	BMA	D	753	2	11,11,12	1.95	4 (36%)	14,15,17	3.40	11 (78%)
2	MAN	D	754	2	11,11,12	0.54	0	14,15,17	1.05	1 (7%)
4	NAG	D	761	1,4	14,14,15	0.37	0	15,19,21	2.23	1 (6%)
4	NAG	D	762	4	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
4	BMA	D	763	4	11,11,12	2.05	4 (36%)	14,15,17	3.48	10 (71%)
2	NAG	E	751	1,2	14,14,15	0.60	0	15,19,21	1.05	1 (6%)
2	NAG	E	752	2	14,14,15	0.66	0	15,19,21	1.71	3 (20%)
2	BMA	E	753	2	11,11,12	2.01	4 (36%)	14,15,17	3.86	10 (71%)
2	MAN	E	754	2	11,11,12	0.63	0	14,15,17	0.78	0
3	NAG	E	761	1,3	14,14,15	0.49	0	15,19,21	2.39	4 (26%)
3	NAG	E	762	3	14,14,15	0.63	1 (7%)	15,19,21	2.62	4 (26%)
3	BMA	E	763	3	11,11,12	1.86	3 (27%)	14,15,17	3.97	8 (57%)
3	MAN	E	764	3	11,11,12	0.56	0	14,15,17	1.18	1 (7%)
3	MAN	E	765	3	11,11,12	0.59	0	14,15,17	0.58	0
2	NAG	F	751	1,2	14,14,15	0.66	0	15,19,21	1.92	2 (13%)
2	NAG	F	752	2	14,14,15	0.47	0	15,19,21	3.35	4 (26%)
2	BMA	F	753	2	11,11,12	2.09	4 (36%)	14,15,17	4.54	10 (71%)
2	MAN	F	754	2	11,11,12	0.49	0	14,15,17	1.43	2 (14%)
3	NAG	F	761	1,3	14,14,15	0.41	0	15,19,21	2.01	3 (20%)
3	NAG	F	762	3	14,14,15	0.43	0	15,19,21	2.24	2 (13%)
3	BMA	F	763	3	11,11,12	2.15	4 (36%)	14,15,17	2.19	7 (50%)
3	MAN	F	764	3	11,11,12	0.59	0	14,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	F	765	3	11,11,12	0.46	0	14,15,17	1.64	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	751	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	752	2	-	0/6/23/26	0/1/1/1
2	BMA	A	753	2	-	0/2/19/22	0/1/1/1
2	MAN	A	754	2	-	0/2/19/22	0/1/1/1
3	NAG	A	761	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	762	3	-	0/6/23/26	0/1/1/1
3	BMA	A	763	3	-	0/2/19/22	0/1/1/1
3	MAN	A	764	3	-	0/2/19/22	0/1/1/1
3	MAN	A	765	3	-	0/2/19/22	1/1/1/1
2	NAG	B	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	752	2	-	0/6/23/26	0/1/1/1
2	BMA	B	753	2	-	0/2/19/22	0/1/1/1
2	MAN	B	754	2	-	0/2/19/22	0/1/1/1
2	NAG	B	761	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	762	2	-	0/6/23/26	0/1/1/1
2	BMA	B	763	2	-	0/2/19/22	0/1/1/1
2	MAN	B	764	2	-	0/2/19/22	0/1/1/1
2	NAG	C	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	752	2	-	0/6/23/26	0/1/1/1
2	BMA	C	753	2	-	0/2/19/22	0/1/1/1
2	MAN	C	754	2	-	0/2/19/22	0/1/1/1
2	NAG	C	761	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	762	2	-	0/6/23/26	0/1/1/1
2	BMA	C	763	2	-	0/2/19/22	0/1/1/1
2	MAN	C	764	2	-	0/2/19/22	1/1/1/1
2	NAG	D	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	752	2	-	0/6/23/26	0/1/1/1
2	BMA	D	753	2	-	0/2/19/22	0/1/1/1
2	MAN	D	754	2	-	0/2/19/22	0/1/1/1
4	NAG	D	761	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	762	4	-	0/6/23/26	0/1/1/1
4	BMA	D	763	4	-	0/2/19/22	0/1/1/1
2	NAG	E	751	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	752	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	E	753	2	-	0/2/19/22	0/1/1/1
2	MAN	E	754	2	-	0/2/19/22	0/1/1/1
3	NAG	E	761	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	762	3	-	0/6/23/26	0/1/1/1
3	BMA	E	763	3	-	0/2/19/22	0/1/1/1
3	MAN	E	764	3	-	0/2/19/22	1/1/1/1
3	MAN	E	765	3	-	0/2/19/22	0/1/1/1
2	NAG	F	751	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	F	752	2	-	1/6/23/26	0/1/1/1
2	BMA	F	753	2	-	0/2/19/22	0/1/1/1
2	MAN	F	754	2	-	0/2/19/22	1/1/1/1
3	NAG	F	761	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	762	3	-	0/6/23/26	0/1/1/1
3	BMA	F	763	3	-	0/2/19/22	0/1/1/1
3	MAN	F	764	3	-	0/2/19/22	0/1/1/1
3	MAN	F	765	3	-	0/2/19/22	1/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	753	BMA	C2-C3	-4.19	1.46	1.52
2	B	753	BMA	C2-C3	-3.40	1.47	1.52
3	F	763	BMA	C2-C3	-3.40	1.47	1.52
2	D	753	BMA	C2-C3	-3.13	1.48	1.52
2	E	753	BMA	C2-C3	-3.10	1.48	1.52

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	753	BMA	C1-O5-C5	-10.24	99.26	112.25
2	F	752	NAG	C4-C3-C2	-9.80	96.00	111.23
3	A	763	BMA	C1-O5-C5	-8.62	101.31	112.25
2	E	753	BMA	C1-O5-C5	-8.25	101.78	112.25
2	B	753	BMA	C1-O5-C5	-7.11	103.23	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	751	NAG	C1
2	F	751	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	752	NAG	C8-C7-N2-C2
2	F	752	NAG	O7-C7-N2-C2
2	E	752	NAG	O7-C7-N2-C2

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	764	MAN	C1-C2-C3-C4-C5-O5
2	C	764	MAN	C1-C2-C3-C4-C5-O5
3	F	765	MAN	C1-C2-C3-C4-C5-O5
3	A	765	MAN	C1-C2-C3-C4-C5-O5
2	F	754	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	751	NAG	1	0
2	A	753	BMA	1	0
2	A	754	MAN	1	0
3	A	762	NAG	1	0
3	A	763	BMA	2	0
3	A	764	MAN	1	0
3	A	765	MAN	1	0
2	B	763	BMA	2	0
2	B	764	MAN	2	0
2	C	751	NAG	2	0
2	C	752	NAG	2	0
2	C	761	NAG	1	0
2	C	762	NAG	1	0
2	C	763	BMA	1	0
2	D	752	NAG	1	0
4	D	761	NAG	2	0
4	D	762	NAG	1	0
3	E	762	NAG	1	0
3	E	763	BMA	1	0
3	F	761	NAG	4	0
3	F	762	NAG	4	0
3	F	765	MAN	2	0

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, 95^{th} 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	613/750 (81%)	0.75	68 (11%)	7 6	52, 123, 277, 384	0
1	B	612/750 (81%)	0.78	69 (11%)	7 5	53, 123, 278, 384	0
1	C	612/750 (81%)	0.76	67 (10%)	7 6	53, 123, 276, 384	0
1	D	612/750 (81%)	0.81	86 (14%)	4 3	52, 123, 275, 384	0
1	E	613/750 (81%)	0.74	76 (12%)	5 4	52, 123, 278, 384	0
1	F	608/750 (81%)	0.77	76 (12%)	5 4	52, 122, 277, 377	0
All	All	3670/4500 (81%)	0.77	442 (12%)	6 5	52, 123, 278, 384	0

The worst 5 of 442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	706	VAL	14.3
1	D	706	VAL	13.7
1	B	720	SER	13.7
1	C	705	HIS	13.5
1	F	705	HIS	11.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MAN	B	754	11/12	0.72	0.59	2.08	164,189,195,195	0
2	MAN	E	754	11/12	0.89	0.52	1.75	191,196,204,207	0
2	MAN	D	754	11/12	0.83	0.38	0.57	176,185,193,194	0
2	MAN	A	754	11/12	0.70	0.31	0.17	225,228,240,247	0
2	MAN	C	754	11/12	0.76	0.31	-0.09	177,187,197,202	0
2	MAN	F	754	11/12	0.85	0.21	-0.71	185,192,197,199	0
2	NAG	F	751	14/15	0.88	0.18	-1.23	78,105,124,134	0
2	NAG	D	751	14/15	0.91	0.17	-1.42	92,103,130,136	0
2	NAG	C	751	14/15	0.90	0.18	-1.61	92,108,127,134	0
2	NAG	B	751	14/15	0.92	0.18	-1.63	91,98,122,133	0
2	NAG	A	751	14/15	0.92	0.15	-2.10	77,100,126,131	0
2	NAG	E	751	14/15	0.90	0.14	-2.28	93,108,125,132	0
3	NAG	F	762	14/15	0.77	0.14	-	199,205,211,212	0
3	MAN	E	765	11/12	0.71	0.26	-	193,208,213,216	0
3	NAG	E	762	14/15	0.75	0.18	-	189,205,217,222	0
3	MAN	A	764	11/12	0.57	0.48	-	176,202,226,228	0
2	NAG	C	761	14/15	0.84	0.17	-	127,150,176,205	0
2	BMA	D	753	11/12	0.80	0.23	-	176,190,223,224	0
2	NAG	B	752	14/15	0.86	0.23	-	113,130,175,175	0
3	BMA	F	763	11/12	0.77	0.17	-	195,209,234,236	0
2	BMA	B	753	11/12	0.83	0.20	-	185,193,201,201	0
2	BMA	C	763	11/12	0.53	0.22	-	138,178,231,243	0
3	BMA	E	763	11/12	0.70	0.18	-	195,214,225,225	0
4	BMA	D	763	11/12	0.75	0.21	-	176,193,202,203	0
3	MAN	A	765	11/12	0.67	0.31	-	174,195,201,207	0
2	NAG	B	762	14/15	0.74	0.20	-	165,190,204,219	0
2	MAN	C	764	11/12	0.59	0.26	-	248,250,254,260	0
2	MAN	B	764	11/12	0.64	0.34	-	244,259,266,268	0
2	BMA	C	753	11/12	0.87	0.13	-	159,180,190,193	0
2	NAG	A	752	14/15	0.84	0.21	-	113,136,144,151	0
3	MAN	F	764	11/12	0.76	0.30	-	241,253,263,265	0
3	MAN	E	764	11/12	0.83	0.29	-	114,174,187,188	0
2	BMA	A	753	11/12	0.89	0.21	-	165,169,197,213	0
3	MAN	F	765	11/12	0.39	0.31	-	209,236,246,247	0
2	NAG	C	752	14/15	0.82	0.33	-	124,164,186,188	0
2	NAG	C	762	14/15	0.70	0.23	-	218,236,246,251	0
2	NAG	B	761	14/15	0.82	0.21	-	144,161,170,183	0
3	NAG	A	761	14/15	0.91	0.19	-	138,164,178,204	0
4	NAG	D	762	14/15	0.84	0.18	-	184,194,201,202	0
2	NAG	F	752	14/15	0.87	0.24	-	98,134,160,166	0
3	NAG	F	761	14/15	0.87	0.16	-	129,152,172,190	0
4	NAG	D	761	14/15	0.82	0.20	-	154,177,186,194	0
2	NAG	D	752	14/15	0.86	0.25	-	110,131,162,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BMA	F	753	11/12	0.84	0.19	-	137,172,188,193	0
3	BMA	A	763	11/12	0.63	0.24	-	194,229,252,253	0
3	NAG	A	762	14/15	0.59	0.25	-	218,228,238,243	0
2	NAG	E	752	14/15	0.93	0.18	-	113,124,164,165	0
2	BMA	E	753	11/12	0.84	0.14	-	173,180,196,200	0
3	NAG	E	761	14/15	0.75	0.24	-	144,163,174,188	0
2	BMA	B	763	11/12	0.80	0.18	-	234,243,255,256	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.