



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2019 – 07:12 PM EST

PDB ID : 5L1X
Title : Structure of the Human Metapneumovirus Fusion Protein in the Postfusion Conformation
Authors : Mas, V.; Melero, J.A.; McLellan, J.S.
Deposited on : 2016-07-29
Resolution : 3.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

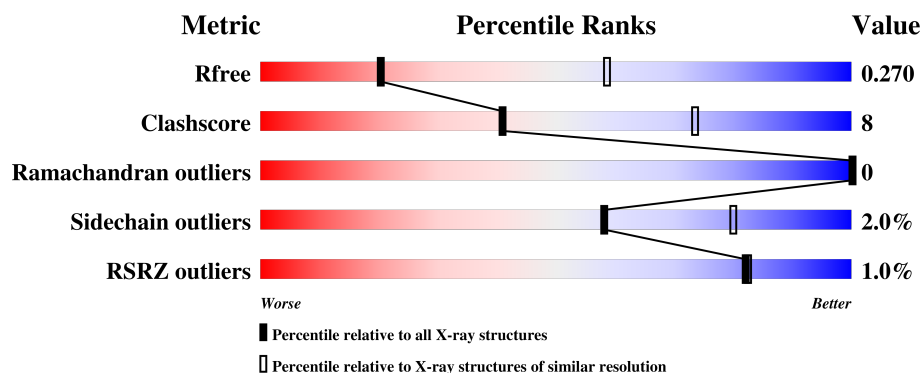
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	89	 60% 21% • 18%
1	C	89	 58% 22% • 18%
1	E	89	 54% 28% 18%
1	G	89	 2% 52% 30% • 17%
1	I	89	 52% 29% • 18%

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Mol	Chain	Length	Quality of chain
1	K	89	
2	B	387	
2	D	387	
2	F	387	
2	H	387	
2	J	387	
2	L	387	

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
3	NAG	C	202	-	-	-	X
3	NAG	L	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20541 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 hMPV F2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	0	0
			568	355	92	119	2			
1	C	73	Total	C	N	O	S	0	0	0
			568	355	92	119	2			
1	E	73	Total	C	N	O	S	0	0	0
			568	355	92	119	2			
1	G	74	Total	C	N	O	S	0	0	0
			577	360	93	122	2			
1	I	73	Total	C	N	O	S	0	0	0
			568	355	92	119	2			
1	K	74	Total	C	N	O	S	0	0	0
			577	360	93	122	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	LYS	-	expression tag	UNP H6X1Z1
A	103	LYS	-	expression tag	UNP H6X1Z1
A	104	ARG	-	expression tag	UNP H6X1Z1
A	105	LYS	-	expression tag	UNP H6X1Z1
A	106	ARG	-	expression tag	UNP H6X1Z1
A	107	ARG	-	expression tag	UNP H6X1Z1
C	102	LYS	-	expression tag	UNP H6X1Z1
C	103	LYS	-	expression tag	UNP H6X1Z1
C	104	ARG	-	expression tag	UNP H6X1Z1
C	105	LYS	-	expression tag	UNP H6X1Z1
C	106	ARG	-	expression tag	UNP H6X1Z1
C	107	ARG	-	expression tag	UNP H6X1Z1
E	102	LYS	-	expression tag	UNP H6X1Z1
E	103	LYS	-	expression tag	UNP H6X1Z1
E	104	ARG	-	expression tag	UNP H6X1Z1
E	105	LYS	-	expression tag	UNP H6X1Z1
E	106	ARG	-	expression tag	UNP H6X1Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	107	ARG	-	expression tag	UNP H6X1Z1
G	102	LYS	-	expression tag	UNP H6X1Z1
G	103	LYS	-	expression tag	UNP H6X1Z1
G	104	ARG	-	expression tag	UNP H6X1Z1
G	105	LYS	-	expression tag	UNP H6X1Z1
G	106	ARG	-	expression tag	UNP H6X1Z1
G	107	ARG	-	expression tag	UNP H6X1Z1
I	102	LYS	-	expression tag	UNP H6X1Z1
I	103	LYS	-	expression tag	UNP H6X1Z1
I	104	ARG	-	expression tag	UNP H6X1Z1
I	105	LYS	-	expression tag	UNP H6X1Z1
I	106	ARG	-	expression tag	UNP H6X1Z1
I	107	ARG	-	expression tag	UNP H6X1Z1
K	102	LYS	-	expression tag	UNP H6X1Z1
K	103	LYS	-	expression tag	UNP H6X1Z1
K	104	ARG	-	expression tag	UNP H6X1Z1
K	105	LYS	-	expression tag	UNP H6X1Z1
K	106	ARG	-	expression tag	UNP H6X1Z1
K	107	ARG	-	expression tag	UNP H6X1Z1

- Molecule 2 is a protein called hMPV F1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	369	Total	C	N	O	S	0	0	0
			2803	1751	491	542	19			
2	D	369	Total	C	N	O	S	0	0	0
			2802	1750	491	542	19			
2	F	369	Total	C	N	O	S	0	0	0
			2803	1751	491	542	19			
2	H	369	Total	C	N	O	S	0	0	0
			2803	1751	491	542	19			
2	J	368	Total	C	N	O	S	0	0	0
			2796	1747	490	540	19			
2	L	370	Total	C	N	O	S	0	0	0
			2809	1754	492	544	19			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	490	SER	-	expression tag	UNP Q8B9P0
B	491	GLY	-	expression tag	UNP Q8B9P0
B	492	ARG	-	expression tag	UNP Q8B9P0

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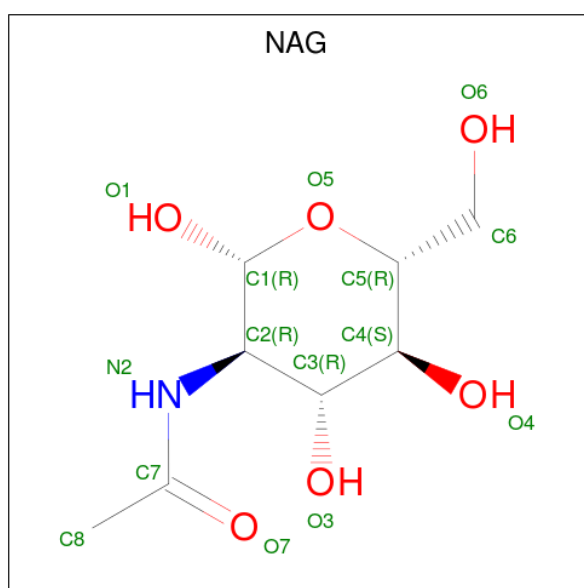
Chain	Residue	Modelled	Actual	Comment	Reference
B	493	GLU	-	expression tag	UNP Q8B9P0
B	494	ASN	-	expression tag	UNP Q8B9P0
B	495	LEU	-	expression tag	UNP Q8B9P0
B	496	TYR	-	expression tag	UNP Q8B9P0
B	497	PHE	-	expression tag	UNP Q8B9P0
B	498	GLN	-	expression tag	UNP Q8B9P0
D	490	SER	-	expression tag	UNP Q8B9P0
D	491	GLY	-	expression tag	UNP Q8B9P0
D	492	ARG	-	expression tag	UNP Q8B9P0
D	493	GLU	-	expression tag	UNP Q8B9P0
D	494	ASN	-	expression tag	UNP Q8B9P0
D	495	LEU	-	expression tag	UNP Q8B9P0
D	496	TYR	-	expression tag	UNP Q8B9P0
D	497	PHE	-	expression tag	UNP Q8B9P0
D	498	GLN	-	expression tag	UNP Q8B9P0
F	490	SER	-	expression tag	UNP Q8B9P0
F	491	GLY	-	expression tag	UNP Q8B9P0
F	492	ARG	-	expression tag	UNP Q8B9P0
F	493	GLU	-	expression tag	UNP Q8B9P0
F	494	ASN	-	expression tag	UNP Q8B9P0
F	495	LEU	-	expression tag	UNP Q8B9P0
F	496	TYR	-	expression tag	UNP Q8B9P0
F	497	PHE	-	expression tag	UNP Q8B9P0
F	498	GLN	-	expression tag	UNP Q8B9P0
H	490	SER	-	expression tag	UNP Q8B9P0
H	491	GLY	-	expression tag	UNP Q8B9P0
H	492	ARG	-	expression tag	UNP Q8B9P0
H	493	GLU	-	expression tag	UNP Q8B9P0
H	494	ASN	-	expression tag	UNP Q8B9P0
H	495	LEU	-	expression tag	UNP Q8B9P0
H	496	TYR	-	expression tag	UNP Q8B9P0
H	497	PHE	-	expression tag	UNP Q8B9P0
H	498	GLN	-	expression tag	UNP Q8B9P0
J	490	SER	-	expression tag	UNP Q8B9P0
J	491	GLY	-	expression tag	UNP Q8B9P0
J	492	ARG	-	expression tag	UNP Q8B9P0
J	493	GLU	-	expression tag	UNP Q8B9P0
J	494	ASN	-	expression tag	UNP Q8B9P0
J	495	LEU	-	expression tag	UNP Q8B9P0
J	496	TYR	-	expression tag	UNP Q8B9P0
J	497	PHE	-	expression tag	UNP Q8B9P0
J	498	GLN	-	expression tag	UNP Q8B9P0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	490	SER	-	expression tag	UNP Q8B9P0
L	491	GLY	-	expression tag	UNP Q8B9P0
L	492	ARG	-	expression tag	UNP Q8B9P0
L	493	GLU	-	expression tag	UNP Q8B9P0
L	494	ASN	-	expression tag	UNP Q8B9P0
L	495	LEU	-	expression tag	UNP Q8B9P0
L	496	TYR	-	expression tag	UNP Q8B9P0
L	497	PHE	-	expression tag	UNP Q8B9P0
L	498	GLN	-	expression tag	UNP Q8B9P0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



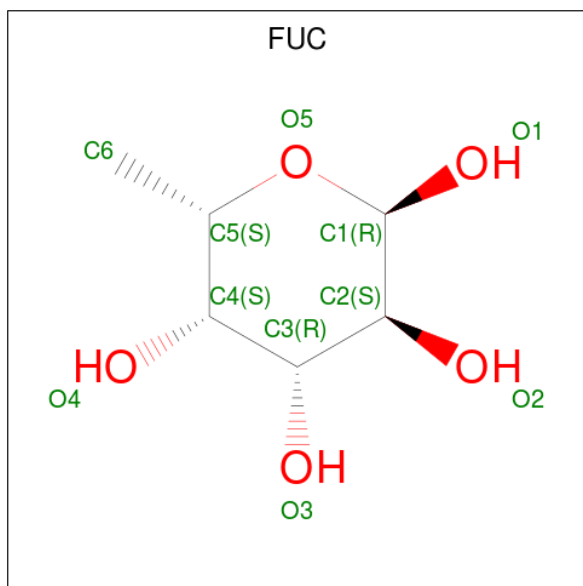
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



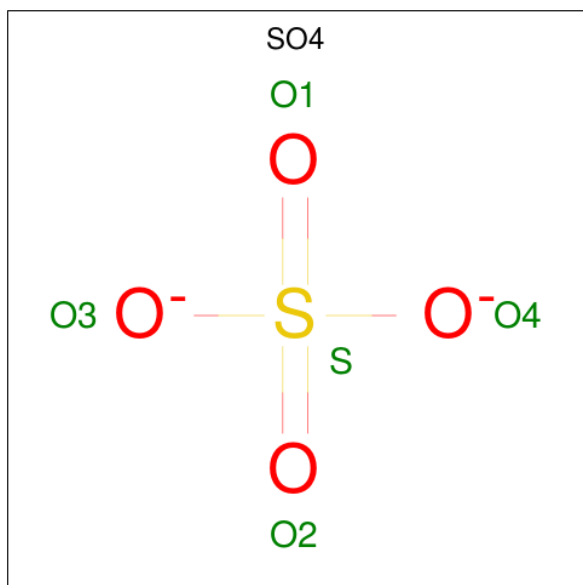
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			10	6	4		
4	H	1	Total	C	O	0	0
			10	6	4		
4	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		

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 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: hMPV F2 subunit

Chain A: 



- Molecule 1: hMPV F2 subunit

Chain C: 



- Molecule 1: hMPV F2 subunit

Chain E: 



ARG

- Molecule 1: hMPV F2 subunit

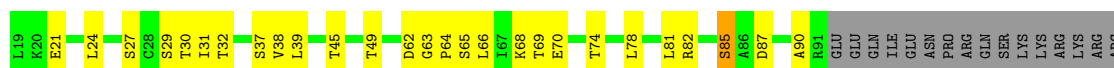
Chain G: 



LYS
ARG
LYS
ARG
ARG

- Molecule 1: hMPV F2 subunit

Chain I: 




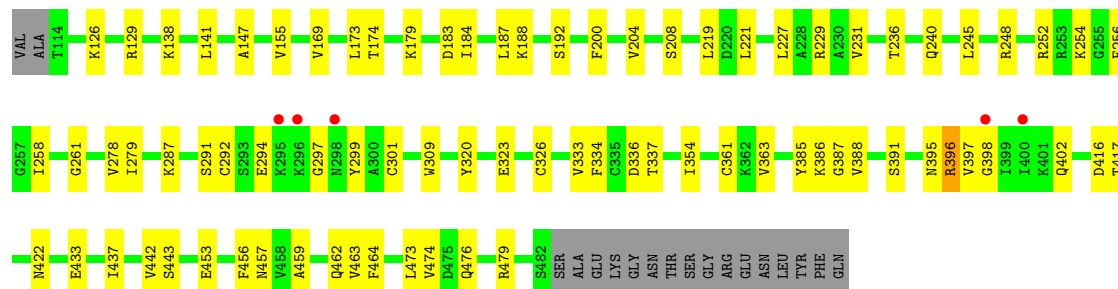
- Molecule 1: hMPV F2 subunit

Chain K: 




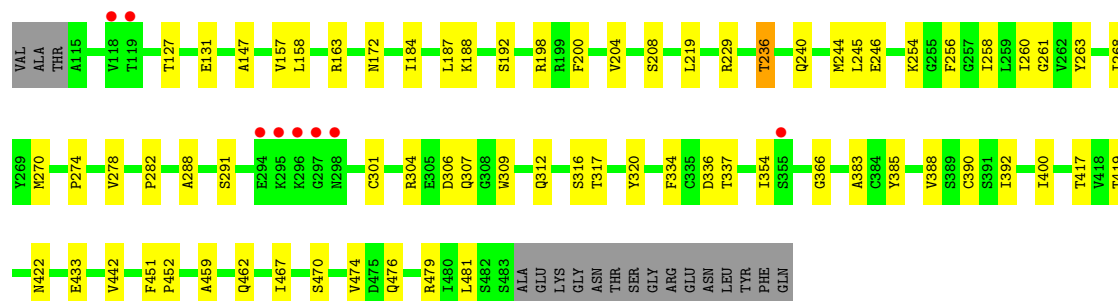
- Molecule 2: hMPV F1 subunit

Chain B: 




- Molecule 2: hMPV F1 subunit

Chain D: 




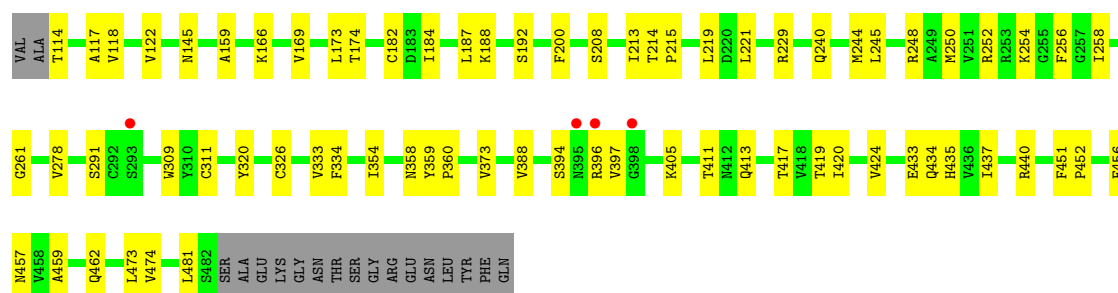
- Molecule 2: hMPV F1 subunit

Chain F: 

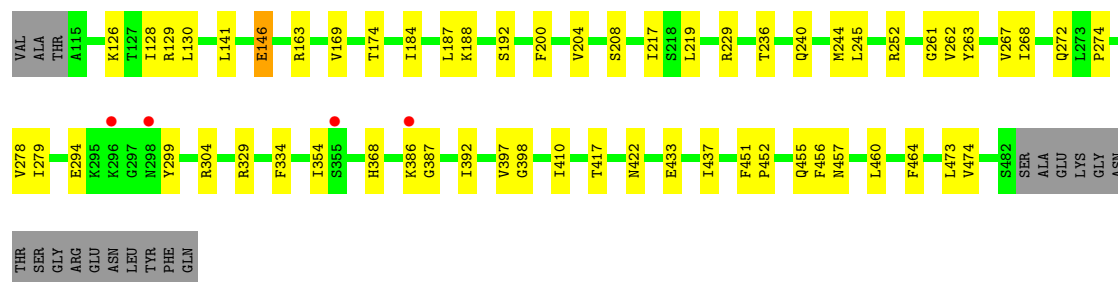
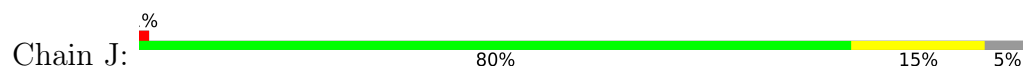


- Molecule 2: hMPV F1 subunit

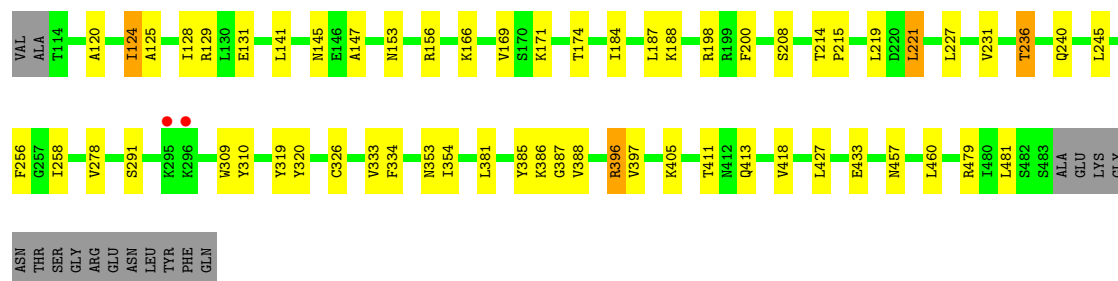
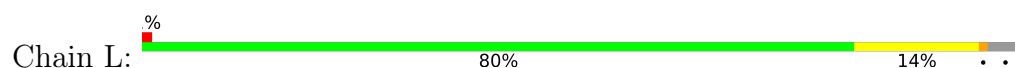
Chain H: 



• Molecule 2: hMPV F1 subunit



• Molecule 2: hMPV F1 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.72Å 128.72Å 572.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.02 – 3.30 37.02 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.02-3.30) 89.6 (37.02-3.30)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.270 0.224 , 0.270	Depositor DCC
R_{free} test set	3677 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20541	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4584e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, SO4, NAG

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	0.37	0/574	0.59	0/779
1	C	0.39	0/574	0.59	0/779
1	E	0.42	0/574	0.61	0/779
1	G	0.39	0/583	0.63	0/791
1	I	0.42	0/574	0.62	0/779
1	K	0.43	0/583	0.64	0/791
2	B	0.39	0/2843	0.56	0/3850
2	D	0.39	0/2842	0.54	1/3848 (0.0%)
2	F	0.39	0/2843	0.55	0/3850
2	H	0.40	0/2843	0.57	0/3850
2	J	0.40	0/2836	0.56	0/3840
2	L	0.42	0/2849	0.57	0/3858
All	All	0.40	0/20518	0.57	1/27794 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	158	LEU	CA-CB-CG	5.27	127.43	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	568	0	564	17	0
1	C	568	0	563	21	0
1	E	568	0	564	20	0
1	G	577	0	570	21	0
1	I	568	0	563	24	0
1	K	577	0	570	19	0
2	B	2803	0	2819	63	0
2	D	2802	0	2818	54	0
2	F	2803	0	2819	44	0
2	H	2803	0	2819	57	0
2	J	2796	0	2813	52	0
2	L	2809	0	2824	49	0
3	B	42	0	37	0	0
3	C	28	0	24	0	0
3	D	14	0	13	1	0
3	F	28	0	25	0	0
3	H	42	0	37	0	0
3	I	14	0	13	0	0
3	J	14	0	13	0	0
3	L	42	0	37	2	0
4	B	10	0	10	0	0
4	C	10	0	10	1	0
4	F	10	0	10	0	0
4	H	10	0	10	0	0
4	L	10	0	10	0	0
5	B	5	0	0	1	0
5	D	5	0	0	1	0
5	F	5	0	0	0	0
5	H	5	0	0	0	0
5	J	5	0	0	0	0
All	All	20541	0	20555	318	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 8.

The worst 5 of 318 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)
2:B:254:LYS:NZ	2:B:336:ASP:OD1	1.98	0.96
1:A:85:SER:HB3	2:B:261:GLY:HA2	1.49	0.94
1:G:85:SER:HB3	2:H:261:GLY:HA2	1.57	0.85
4:C:203:FUC:O3	2:L:479:ARG:NH1	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:GLN:HE21	2:J:329:ARG:HH12	1.25	0.81

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	71/89 (80%)	69 (97%)	2 (3%)	0	100	100
1	C	71/89 (80%)	69 (97%)	2 (3%)	0	100	100
1	E	71/89 (80%)	69 (97%)	2 (3%)	0	100	100
1	G	72/89 (81%)	71 (99%)	1 (1%)	0	100	100
1	I	71/89 (80%)	69 (97%)	2 (3%)	0	100	100
1	K	72/89 (81%)	71 (99%)	1 (1%)	0	100	100
2	B	367/387 (95%)	357 (97%)	10 (3%)	0	100	100
2	D	367/387 (95%)	358 (98%)	9 (2%)	0	100	100
2	F	367/387 (95%)	360 (98%)	7 (2%)	0	100	100
2	H	367/387 (95%)	357 (97%)	10 (3%)	0	100	100
2	J	366/387 (95%)	356 (97%)	10 (3%)	0	100	100
2	L	368/387 (95%)	362 (98%)	6 (2%)	0	100	100
All	All	2630/2856 (92%)	2568 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	65/81 (80%)	64 (98%)	1 (2%)	67	84
1	C	65/81 (80%)	64 (98%)	1 (2%)	67	84
1	E	65/81 (80%)	65 (100%)	0	100	100
1	G	66/81 (82%)	63 (96%)	3 (4%)	30	64
1	I	65/81 (80%)	63 (97%)	2 (3%)	43	72
1	K	66/81 (82%)	66 (100%)	0	100	100
2	B	312/326 (96%)	305 (98%)	7 (2%)	55	79
2	D	312/326 (96%)	306 (98%)	6 (2%)	60	80
2	F	312/326 (96%)	306 (98%)	6 (2%)	60	80
2	H	312/326 (96%)	306 (98%)	6 (2%)	60	80
2	J	311/326 (95%)	304 (98%)	7 (2%)	53	78
2	L	313/326 (96%)	307 (98%)	6 (2%)	60	80
All	All	2264/2442 (93%)	2219 (98%)	45 (2%)	58	80

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	457	ASN
2	H	245	LEU
2	L	236	THR
1	G	30	THR
2	H	311	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	88	GLN
2	H	435	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

26 ligands 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	$\# Z > 2$
3	NAG	B	501	2	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
3	NAG	B	502	3,2,4	14,14,15	0.99	1 (7%)	17,19,21	0.77	0
3	NAG	B	503	3	14,14,15	0.38	0	17,19,21	0.40	0
4	FUC	B	504	3	9,10,11	0.37	0	13,14,16	1.04	1 (7%)
5	SO4	B	505	-	4,4,4	0.19	0	6,6,6	0.16	0
3	NAG	C	201	1,3,4	14,14,15	1.38	2 (14%)	17,19,21	1.36	3 (17%)
3	NAG	C	202	3	14,14,15	0.97	1 (7%)	17,19,21	1.12	1 (5%)
4	FUC	C	203	3	9,10,11	0.50	0	13,14,16	1.24	2 (15%)
3	NAG	D	501	2	14,14,15	0.65	1 (7%)	17,19,21	0.47	0
5	SO4	D	502	-	4,4,4	0.17	0	6,6,6	0.14	0
3	NAG	F	501	2	14,14,15	0.52	0	17,19,21	0.66	0
3	NAG	F	502	2,4	14,14,15	0.41	0	17,19,21	0.59	0
4	FUC	F	503	3	9,10,11	0.92	0	13,14,16	2.14	6 (46%)
5	SO4	F	504	-	4,4,4	0.17	0	6,6,6	0.14	0
3	NAG	H	501	3,2	14,14,15	0.52	0	17,19,21	0.58	0
3	NAG	H	502	3	14,14,15	0.50	0	17,19,21	0.41	0
3	NAG	H	503	2,4	14,14,15	0.47	0	17,19,21	0.56	0
4	FUC	H	504	3	9,10,11	0.39	0	13,14,16	0.64	0
5	SO4	H	505	-	4,4,4	0.15	0	6,6,6	0.09	0
3	NAG	I	201	1	14,14,15	0.90	1 (7%)	17,19,21	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	501	2	14,14,15	0.42	0	17,19,21	0.48	0
5	SO4	J	502	-	4,4,4	0.14	0	6,6,6	0.24	0
3	NAG	L	501	2	14,14,15	0.46	0	17,19,21	0.38	0
3	NAG	L	502	3,2,4	14,14,15	1.41	1 (7%)	17,19,21	0.97	1 (5%)
3	NAG	L	503	3	14,14,15	0.47	0	17,19,21	1.06	1 (5%)
4	FUC	L	504	3	9,10,11	0.55	0	13,14,16	1.59	3 (23%)

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
3	NAG	B	501	2	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,2,4	-	0/6/23/26	0/1/1/1
3	NAG	B	503	3	-	2/6/23/26	0/1/1/1
4	FUC	B	504	3	-	-	0/1/1/1
3	NAG	C	201	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	C	202	3	-	2/6/23/26	0/1/1/1
4	FUC	C	203	3	-	-	0/1/1/1
3	NAG	D	501	2	-	2/6/23/26	0/1/1/1
3	NAG	F	501	2	-	0/6/23/26	0/1/1/1
3	NAG	F	502	2,4	-	0/6/23/26	0/1/1/1
4	FUC	F	503	3	-	-	0/1/1/1
3	NAG	H	501	3,2	-	0/6/23/26	0/1/1/1
3	NAG	H	502	3	-	2/6/23/26	0/1/1/1
3	NAG	H	503	2,4	-	0/6/23/26	0/1/1/1
4	FUC	H	504	3	-	-	0/1/1/1
3	NAG	I	201	1	-	0/6/23/26	0/1/1/1
3	NAG	J	501	2	-	0/6/23/26	0/1/1/1
3	NAG	L	501	2	-	0/6/23/26	0/1/1/1
3	NAG	L	502	3,2,4	-	0/6/23/26	0/1/1/1
3	NAG	L	503	3	-	3/6/23/26	0/1/1/1
4	FUC	L	504	3	-	-	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	502	NAG	O5-C1	-5.03	1.35	1.43
3	C	201	NAG	O5-C1	3.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAG	O5-C1	-3.55	1.38	1.43
3	C	201	NAG	C1-C2	3.37	1.57	1.52
3	C	202	NAG	C1-C2	3.35	1.57	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	201	NAG	C1-O5-C5	4.13	117.82	112.20
3	C	202	NAG	C1-O5-C5	3.93	117.55	112.20
4	L	504	FUC	C1-C2-C3	3.70	114.21	109.66
4	F	503	FUC	O5-C1-C2	3.65	116.42	110.79
3	L	503	NAG	C2-N2-C7	3.57	128.03	122.92

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	503	NAG	C3-C2-N2-C7
3	B	503	NAG	O5-C5-C6-O6
3	L	503	NAG	O5-C5-C6-O6
3	L	503	NAG	C4-C5-C6-O6
3	B	503	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	203	FUC	1	0
3	D	501	NAG	1	0
3	L	502	NAG	1	0
3	L	503	NAG	2	0

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	73/89 (82%)	-0.23	0 100 100	48, 78, 118, 131	0
1	C	73/89 (82%)	-0.32	0 100 100	42, 71, 114, 133	0
1	E	73/89 (82%)	-0.22	0 100 100	44, 66, 108, 127	0
1	G	74/89 (83%)	-0.25	2 (2%) 54 53	46, 71, 117, 128	0
1	I	73/89 (82%)	-0.43	0 100 100	42, 64, 104, 120	0
1	K	74/89 (83%)	-0.23	0 100 100	48, 65, 113, 133	0
2	B	369/387 (95%)	-0.22	5 (1%) 75 74	42, 84, 117, 153	0
2	D	369/387 (95%)	-0.20	8 (2%) 62 61	38, 81, 121, 153	0
2	F	369/387 (95%)	-0.38	2 (0%) 90 90	43, 71, 105, 125	0
2	H	369/387 (95%)	-0.23	4 (1%) 80 81	35, 75, 110, 149	0
2	J	368/387 (95%)	-0.25	4 (1%) 80 81	40, 71, 116, 159	0
2	L	370/387 (95%)	-0.41	2 (0%) 90 90	42, 66, 97, 123	0
All	All	2654/2856 (92%)	-0.28	27 (1%) 82 82	35, 74, 115, 159	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	296	LYS	3.8
2	H	398	GLY	3.6
2	J	296	LYS	3.5
2	J	298	ASN	3.2
2	F	296	LYS	3.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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
3	NAG	L	503	14/15	0.71	0.45	128,139,147,149	0
3	NAG	F	502	14/15	0.74	0.28	100,117,124,125	0
3	NAG	D	501	14/15	0.78	0.35	86,112,118,121	0
3	NAG	I	201	14/15	0.78	0.26	88,100,113,113	0
3	NAG	C	202	14/15	0.79	0.52	123,127,129,129	0
3	NAG	H	502	14/15	0.80	0.34	115,120,124,124	0
3	NAG	B	503	14/15	0.81	0.53	129,133,137,138	0
3	NAG	H	503	14/15	0.81	0.31	102,112,116,117	0
4	FUC	C	203	10/11	0.82	0.42	104,109,112,114	0
4	FUC	L	504	10/11	0.83	0.34	110,121,126,131	0
4	FUC	B	504	10/11	0.83	0.48	129,134,137,137	0
5	SO4	F	504	5/5	0.84	0.28	138,139,140,141	0
3	NAG	L	502	14/15	0.84	0.19	102,109,117,126	0
3	NAG	F	501	14/15	0.85	0.15	80,98,101,102	0
3	NAG	B	502	14/15	0.86	0.35	104,117,123,127	0
3	NAG	B	501	14/15	0.86	0.18	58,73,88,92	0
3	NAG	C	201	14/15	0.87	0.48	85,119,124,124	0
3	NAG	J	501	14/15	0.89	0.34	73,90,104,106	0
5	SO4	B	505	5/5	0.91	0.20	112,113,118,118	0
3	NAG	L	501	14/15	0.91	0.17	73,88,100,102	0
4	FUC	H	504	10/11	0.92	0.30	109,115,117,118	0
5	SO4	H	505	5/5	0.92	0.16	118,122,122,123	0
3	NAG	H	501	14/15	0.93	0.14	65,77,86,102	0
5	SO4	J	502	5/5	0.95	0.17	99,100,102,102	0
4	FUC	F	503	10/11	0.95	0.38	125,127,132,132	0
5	SO4	D	502	5/5	0.96	0.09	103,103,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.