W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 06:30 PM EDT

PDB ID	:	5FVC
Title	:	Structure of RNA-bound decameric HMPV nucleoprotein
Authors	:	Renner, M.; Bertinelli, M.; Leyrat, C.; Paesen, G.C.; Saraiva de Oliveira, L.F.; Huiskonen, J.T.; Grimes, J.M.
Deposited on	:	2016-02-05
Resolution	:	4.17 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

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 4.17 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.
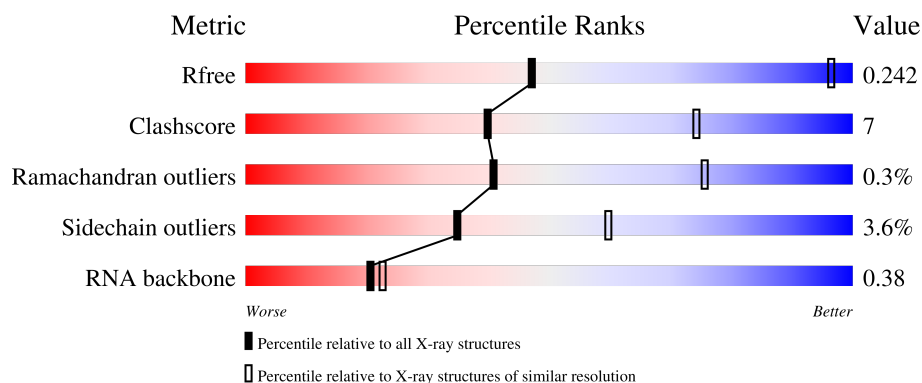
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1034 (4.60-3.76)
Clashscore	141614	1030 (4.54-3.80)
Ramachandran outliers	138981	1006 (4.58-3.78)
Sidechain outliers	138945	1037 (4.60-3.76)
RNA backbone	3102	1049 (5.04-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	401	68% 17% • 14%
1	B	401	72% 18% • 8%
1	C	401	68% 18% • 14%
1	D	401	73% 18% • 8%
1	E	401	72% 18% • 9%
1	F	401	72% 18% • 9%

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Mol	Chain	Length	Quality of chain
1	G	401	74% 17% · 8%
1	H	401	68% 18% · 12%
1	I	401	73% 18% · 9%
1	J	401	72% 18% · 9%
2	K	70	17% 50% 30% ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 29357 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 NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2679	1693	466	510	10			
1	B	367	Total	C	N	O	S	0	0	0
			2848	1801	492	544	11			
1	C	346	Total	C	N	O	S	0	0	0
			2682	1696	466	509	11			
1	D	369	Total	C	N	O	S	0	0	0
			2863	1809	495	548	11			
1	E	364	Total	C	N	O	S	0	0	0
			2815	1775	489	541	10			
1	F	366	Total	C	N	O	S	0	0	0
			2838	1793	491	544	10			
1	G	368	Total	C	N	O	S	0	0	0
			2850	1797	494	548	11			
1	H	351	Total	C	N	O	S	0	0	0
			2719	1718	473	517	11			
1	I	366	Total	C	N	O	S	0	0	0
			2834	1788	490	545	11			
1	J	364	Total	C	N	O	S	0	0	0
			2829	1790	489	539	11			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	LYS	-	expression tag	UNP Q91F57
A	396	HIS	-	expression tag	UNP Q91F57
A	397	HIS	-	expression tag	UNP Q91F57
A	398	HIS	-	expression tag	UNP Q91F57
A	399	HIS	-	expression tag	UNP Q91F57
A	400	HIS	-	expression tag	UNP Q91F57
A	401	HIS	-	expression tag	UNP Q91F57
B	395	LYS	-	expression tag	UNP Q91F57
B	396	HIS	-	expression tag	UNP Q91F57

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Chain	Residue	Modelled	Actual	Comment	Reference
B	397	HIS	-	expression tag	UNP Q91F57
B	398	HIS	-	expression tag	UNP Q91F57
B	399	HIS	-	expression tag	UNP Q91F57
B	400	HIS	-	expression tag	UNP Q91F57
B	401	HIS	-	expression tag	UNP Q91F57
C	395	LYS	-	expression tag	UNP Q91F57
C	396	HIS	-	expression tag	UNP Q91F57
C	397	HIS	-	expression tag	UNP Q91F57
C	398	HIS	-	expression tag	UNP Q91F57
C	399	HIS	-	expression tag	UNP Q91F57
C	400	HIS	-	expression tag	UNP Q91F57
C	401	HIS	-	expression tag	UNP Q91F57
D	395	LYS	-	expression tag	UNP Q91F57
D	396	HIS	-	expression tag	UNP Q91F57
D	397	HIS	-	expression tag	UNP Q91F57
D	398	HIS	-	expression tag	UNP Q91F57
D	399	HIS	-	expression tag	UNP Q91F57
D	400	HIS	-	expression tag	UNP Q91F57
D	401	HIS	-	expression tag	UNP Q91F57
E	395	LYS	-	expression tag	UNP Q91F57
E	396	HIS	-	expression tag	UNP Q91F57
E	397	HIS	-	expression tag	UNP Q91F57
E	398	HIS	-	expression tag	UNP Q91F57
E	399	HIS	-	expression tag	UNP Q91F57
E	400	HIS	-	expression tag	UNP Q91F57
E	401	HIS	-	expression tag	UNP Q91F57
F	395	LYS	-	expression tag	UNP Q91F57
F	396	HIS	-	expression tag	UNP Q91F57
F	397	HIS	-	expression tag	UNP Q91F57
F	398	HIS	-	expression tag	UNP Q91F57
F	399	HIS	-	expression tag	UNP Q91F57
F	400	HIS	-	expression tag	UNP Q91F57
F	401	HIS	-	expression tag	UNP Q91F57
G	395	LYS	-	expression tag	UNP Q91F57
G	396	HIS	-	expression tag	UNP Q91F57
G	397	HIS	-	expression tag	UNP Q91F57
G	398	HIS	-	expression tag	UNP Q91F57
G	399	HIS	-	expression tag	UNP Q91F57
G	400	HIS	-	expression tag	UNP Q91F57
G	401	HIS	-	expression tag	UNP Q91F57
H	395	LYS	-	expression tag	UNP Q91F57
H	396	HIS	-	expression tag	UNP Q91F57

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Chain	Residue	Modelled	Actual	Comment	Reference
H	397	HIS	-	expression tag	UNP Q91F57
H	398	HIS	-	expression tag	UNP Q91F57
H	399	HIS	-	expression tag	UNP Q91F57
H	400	HIS	-	expression tag	UNP Q91F57
H	401	HIS	-	expression tag	UNP Q91F57
I	395	LYS	-	expression tag	UNP Q91F57
I	396	HIS	-	expression tag	UNP Q91F57
I	397	HIS	-	expression tag	UNP Q91F57
I	398	HIS	-	expression tag	UNP Q91F57
I	399	HIS	-	expression tag	UNP Q91F57
I	400	HIS	-	expression tag	UNP Q91F57
I	401	HIS	-	expression tag	UNP Q91F57
J	395	LYS	-	expression tag	UNP Q91F57
J	396	HIS	-	expression tag	UNP Q91F57
J	397	HIS	-	expression tag	UNP Q91F57
J	398	HIS	-	expression tag	UNP Q91F57
J	399	HIS	-	expression tag	UNP Q91F57
J	400	HIS	-	expression tag	UNP Q91F57
J	401	HIS	-	expression tag	UNP Q91F57

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	K	70	1400	630	210	490	70	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues a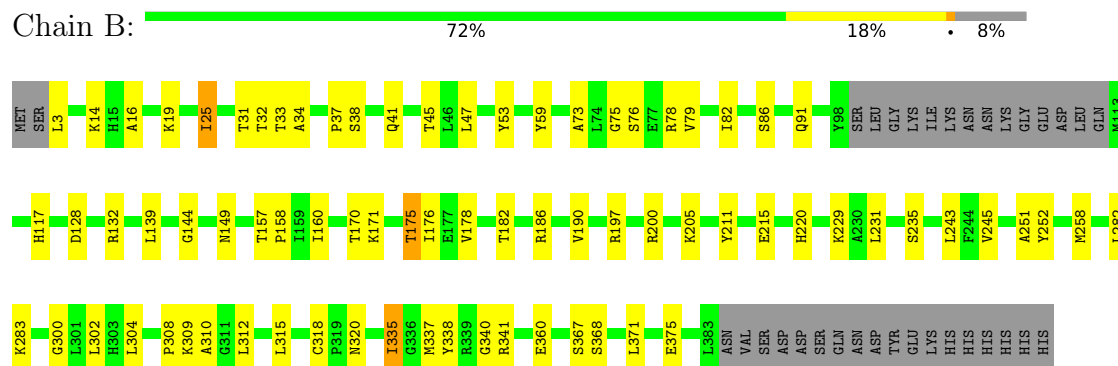re color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
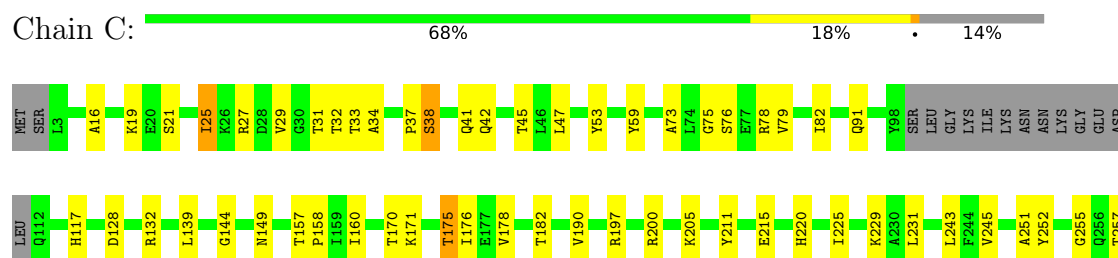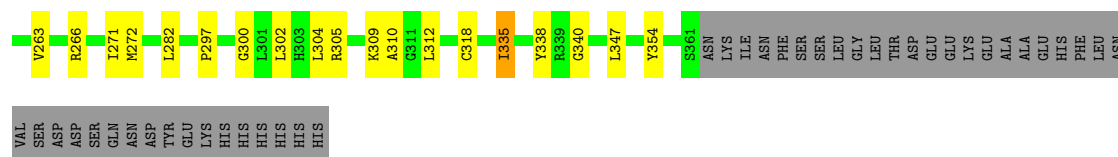
- Molecule 1: HMPV NUCLEOPROTEIN

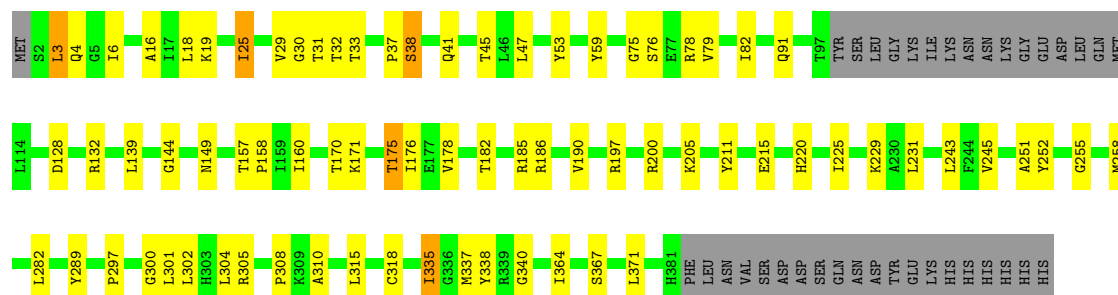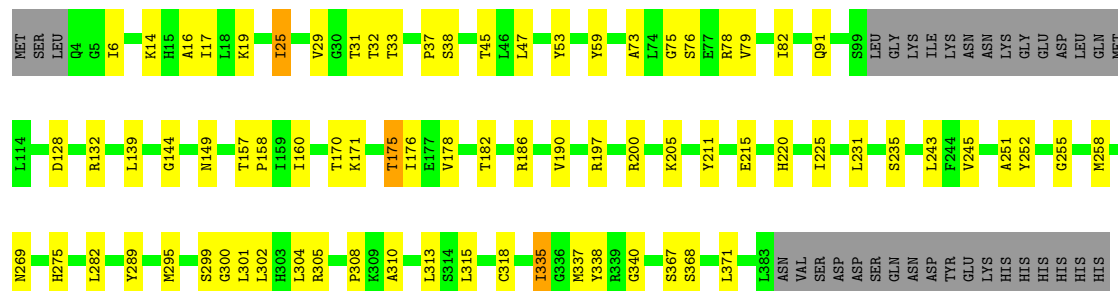Chain A:

68%   17%   •   14%

- Molecule 1: HMPV NUCLEOPROTEIN

Chain B:

72%   18%   •   8%

- Molecule 1: HMPV NUCLEOPROTEIN

Chain C:

68%   18%   •   14%

V263 R266 I271 M272 L282 P297 G300 L301 L302 H303 L304 R305 K309 A310 G311 L312 C318 I335 Y338 R339 G340 L347 Y354 S361 ASN LYS ILE ASN PHE SER SER LEU GLY LEU THR ASP GLU GLU LYS GLU ALA ALA GLU HIS PHE LEU ASN

VAL SER ASP ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 1: HMPV NUCLEOPROTEIN

Chain D: 73%   18%   •   8%

MET S2 L3 I6 A16 I17 L18 K19 E20 S21 I25 V29 G30 T31 T32 T33 P37 S38 Q41 Q42 T45 L46 L47 Y53 A57 D58 Y59 A73 L74 G75 S76 E77 R78 V79 I82 Q91 Y98 SER LEU GLY LYS ILE LYS ASN ASN LYS GLY

GLU ASP LEU Q112 D128 R132 L139 G144 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R186 V190 R197 R200 P204 K205 Y211 E215 H220 I225 L231 G232 S235 T236 G237 L243 F244 V245

A251 Y252 G255 M258 V263 R266 L282 G300 L301 L302 H303 L304 R305 A310 L315 C318 I335 Y338 R339 G340 S367 L383 ASN VAL SER ASP ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 1: HMPV NUCLEOPROTEIN

Chain E: 72%   18%   •   9%

MET S2 L3 Q4 G5 I6 A16 I17 L18 K19 I25 V29 G30 T31 T32 T33 P37 S38 Q41 T45 L46 L47 Y53 Y59 G75 S76 E77 R78 V79 I82 Q91 T97 TYR SER LEU GLY LYS ILE LYS ASN ASN LYS GLY GLU ASP LEU GLN MET

L114 D128 R132 L139 G144 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R185 R186 V190 R197 R200 K205 Y211 E215 H220 I225 K229 A230 L231 L243 F244 V245 A251 Y252 G255 M258

L282 Y289 P297 G300 L301 L302 H303 L304 R305 P308 K309 A310 L315 C318 I335 G336 M337 Y338 R339 G340 I364 S367 L371 H381 PHE LEU ASN VAL SER ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 1: HMPV NUCLEOPROTEIN

Chain F: 72%   18%   •   9%

MET SER LEU Q4 G5 I6 K14 H15 A16 I17 L18 K19 I25 V29 G30 T31 T32 T33 P37 S38 T45 L46 L47 Y53 Y59 A73 L74 G75 S76 E77 R78 V79 I82 Q91 S99 LEU GLY LYS ILE LYS ASN ASN LYS GLY GLU ASP LEU GLN MET

L114 D128 R132 L139 G144 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R186 V190 R197 R200 K205 Y211 E215 H220 I225 L231 S235 L243 F244 V245 A251 Y252 G255 M258

N269 H275 L282 Y289 M295 S299 G300 L301 L302 H303 L304 R305 P308 K309 A310 L313 S314 L315 C318 I335 G336 M337 Y338 R339 G340 S367 S368 L371 L383 ASN VAL SER ASP ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 1: HMPV NUCLEOPROTEIN

Chain G: 74%   17%   •   8%

MET S2 I6 K14 H15 A16 K19 I25 V29 G30 T31 T32 T33 A34 P37 S38 T45 L46 L47 Y53 Y59 G75 S76 E77 R78 V79 I82 Q91 S99 LEU GLY LYS ILE LYS ASN ASN LYS GLY GLU ASP LEU Q112 H117 D128

R132 L139 G144 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R186 V190 R197 R200 K205 Y211 E215 H220 I225 K229 A230 L231 L243 F244 V245 A251 Y252 T257 M258 R266 N269 L282

R293 P297 G300 L301 L302 H303 L304 R305 P308 K309 A310 L315 C318 I335 G336 M337 Y338 R339 G340 S367 L371 H381 PHE LEU ASN VAL SER ASP ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: HMPV NUCLEOPROTEIN

Chain H: 68% 18% • 12%

MET S2 L3 Q4 G5 I6 H7 V13 K14 H15 A16 I17 L18 K19 I25 K26 R27 D28 V29 G30 T31 T32 T33 P37 S38 Q41 T45 L46 L47 Y53 Y59 A73 L74 G75 S76 E77 R78 V79 I82 Q91 S99 LEU GLY LYS ILE LYS ASN ASN LYS

GLY GLU ASP LEU Q112 D128 R132 L139 G144 N145 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R186 V190 R197 R200 K205 Y211 E215 H220 I225 K229 A230 L231 K239 L243 F244 V245

A251 Y252 M258 N269 N270 I271 L282 Y289 R293 P297 G300 L301 L302 H303 L304 R305 A310 L315 C318 I335 Y338 R339 G340 I364 ASN PHE SER SER LEU GLY LEU THR ASP GLU GLU LYS GLU ALA ALA GLU HIS PHE LEU ASN VAL SER ASP

ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: HMPV NUCLEOPROTEIN

Chain I: 73% 18% • 9%

MET SER L3 I6 H7 Y13 A16 I17 L18 K19 E20 S21 I25 V29 G30 T31 T32 T33 A34 P37 S38 Q41 T45 L46 L47 Y53 Y59 A73 L74 G75 S76 E77 R78 V79 I82 Q91 S99 LEU GLY LYS ILE LYS ASN ASN LYS GLY

GLU ASP LEU Q112 H117 D128 R132 L139 G144 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R186 V190 R197 R200 K205 Y211 E215 H220 K229 A230 L231 L243 F244 V245 A251 Y252 T257

M258 W261 R266 L282 G300 L301 L302 H303 L304 R305 Q306 S307 P308 K309 A310 L315 C318 I335 Y338 R339 G340 I364 S367 A379 E380 HIS PHE LEU ASN VAL SER ASP ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: HMPV NUCLEOPROTEIN

Chain J: 72% 18% • 9%

MET SER L3 I6 A16 K19 E20 S21 I25 V29 G30 T31 T32 T33 A34 P37 S38 Q41 T45 L46 L47 Y53 Y59 G75 S76 E77 R78 V79 I82 Q91 S99 LEU GLY LYS ILE LYS ASN ASN LYS GLY GLU ASP LEU Q112 M113 L114

H117 D128 R132 L139 LYS GLU SER SER GLY N145 N149 T157 P158 I159 I160 T170 K171 T175 I176 E177 V178 T182 R185 R186 V190 R197 R200 K205 Y211 E215 H220 I225 K229 A230 L231 L243 F244 V245 A251

Y252 M258 R266 I271 H275 Q279 L282 G300 L301 L302 H303 L304 R305 P308 K309 A310 G311 L312 L315 C318 I335 G336 M337 Y338 R339 G340 E360 S367 L371 L383 ASN VAL SER ASP ASP SER GLN ASN ASP TYR GLU LYS HIS HIS HIS

HIS HIS HIS

● Molecule 2: RNA

Chain K:

17%   50%   30%

C1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C12 C13 C14 C15 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C32 C33 C34 C35 C36 C37 C38 C39 C40 C41 C42 C43 C44 C45 C46 C47 C48 C49 C50 C51 C54 C55 C56 C57 C58 C59 C60 C61 C62 C63

C64 C65 C66 C67 C68 C69 C70

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	202.01Å 233.21Å 203.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.19 – 4.17 101.19 – 4.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (101.19-4.17) 99.9 (101.19-4.17)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.41 (at 4.15Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.191 , 0.230 0.212 , 0.242	Depositor DCC
R_{free} test set	1798 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	189.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 254.7	EDS
L-test for twinning [2]	$<|L|> = 0.44$, $<L^2> = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	29357	wwPDB-VP
Average B, all atoms (Å^2)	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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	0.47	0/2722	0.68	0/3678
1	B	0.45	0/2894	0.68	0/3908
1	C	0.45	0/2725	0.66	0/3681
1	D	0.47	0/2909	0.69	0/3928
1	E	0.46	0/2859	0.68	0/3861
1	F	0.45	0/2884	0.68	0/3895
1	G	0.45	0/2895	0.68	0/3909
1	H	0.46	0/2762	0.69	1/3730 (0.0%)
1	I	0.47	0/2878	0.68	1/3886 (0.0%)
1	J	0.51	1/2874 (0.0%)	0.71	3/3881 (0.1%)
2	K	1.61	21/1539 (1.4%)	1.02	0/2376
All	All	0.58	22/29941 (0.1%)	0.71	5/40733 (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	B	0	1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	47	LEU	CG-CD1	9.19	1.85	1.51
2	K	7	C	C1'-N1	8.28	1.61	1.48
2	K	28	C	C1'-N1	7.26	1.59	1.48
2	K	14	C	C1'-N1	7.00	1.59	1.48
2	K	42	C	C1'-N1	6.91	1.59	1.48

All (5) bond angle outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	47	LEU	CD1-CG-CD2	-11.03	77.43	110.50
1	J	47	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	H	25	ILE	CB-CA-C	-5.98	99.65	111.60
1	I	306	GLN	CG-CD-OE1	5.38	132.37	121.60
1	J	47	LEU	CB-CG-CD1	-5.10	102.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	320	ASN	Sidechain

5.2 Too-close contacts ⓘ

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	2679	0	2731	44	2
1	B	2848	0	2894	45	0
1	C	2682	0	2737	48	0
1	D	2863	0	2907	53	2
1	E	2815	0	2861	56	0
1	F	2838	0	2879	52	0
1	G	2850	0	2892	48	0
1	H	2719	0	2777	54	1
1	I	2834	0	2880	54	0
1	J	2829	0	2874	58	0
2	K	1400	0	770	42	0
All	All	29357	0	29202	427	3

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 7.

The worst 5 of 427 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:J:47:LEU:CG	1:J:47:LEU:CD1	1.85	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:LEU:CD1	1:J:47:LEU:CD2	2.14	1.24
1:A:3:LEU:HD23	1:J:282:LEU:HD11	1.31	1.11
1:E:41:GLN:HB3	1:F:29:VAL:HG11	1.31	1.07
1:I:41:GLN:HB3	1:J:29:VAL:HG11	1.39	1.04

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:MET:SD	1:D:57:ALA:O[7_747]	1.93	0.27
1:A:177:GLU:OE2	1:D:204:PRO:CG[7_747]	2.01	0.19
1:H:145:ASN:OD1	1:H:145:ASN:OD1[4_557]	2.02	0.18

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/401 (85%)	321 (94%)	20 (6%)	1 (0%)	41	75
1	B	363/401 (90%)	342 (94%)	20 (6%)	1 (0%)	41	75
1	C	342/401 (85%)	321 (94%)	20 (6%)	1 (0%)	41	75
1	D	365/401 (91%)	342 (94%)	22 (6%)	1 (0%)	41	75
1	E	360/401 (90%)	337 (94%)	22 (6%)	1 (0%)	41	75
1	F	362/401 (90%)	341 (94%)	20 (6%)	1 (0%)	41	75
1	G	364/401 (91%)	343 (94%)	20 (6%)	1 (0%)	41	75
1	H	347/401 (86%)	325 (94%)	21 (6%)	1 (0%)	41	75
1	I	362/401 (90%)	341 (94%)	20 (6%)	1 (0%)	41	75
1	J	358/401 (89%)	336 (94%)	21 (6%)	1 (0%)	41	75
All	All	3565/4010 (89%)	3349 (94%)	206 (6%)	10 (0%)	41	75

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ILE
1	B	335	ILE
1	D	335	ILE
1	E	335	ILE
1	F	335	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/343 (85%)	282 (96%)	11 (4%)	33	58
1	B	311/343 (91%)	300 (96%)	11 (4%)	36	60
1	C	293/343 (85%)	284 (97%)	9 (3%)	40	62
1	D	313/343 (91%)	301 (96%)	12 (4%)	33	58
1	E	308/343 (90%)	296 (96%)	12 (4%)	32	57
1	F	310/343 (90%)	298 (96%)	12 (4%)	32	57
1	G	312/343 (91%)	301 (96%)	11 (4%)	36	60
1	H	298/343 (87%)	288 (97%)	10 (3%)	37	60
1	I	310/343 (90%)	300 (97%)	10 (3%)	39	62
1	J	309/343 (90%)	298 (96%)	11 (4%)	35	60
All	All	3057/3430 (89%)	2948 (96%)	109 (4%)	35	60

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	SER
1	G	47	LEU
1	J	31	THR
1	F	175	THR
1	F	335	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11

such sidechains are listed below:

Mol	Chain	Res	Type
1	G	320	ASN
1	H	320	ASN
1	J	320	ASN
1	I	320	ASN
1	D	320	ASN

5.3.3   RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	K	69/70 (98%)	23 (33%)	7 (10%)

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	K	4	C
2	K	8	C
2	K	11	C
2	K	12	C
2	K	15	C

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	K	32	C
2	K	39	C
2	K	67	C
2	K	46	C
2	K	25	C

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3　Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4　Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5　Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.