



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:48 pm BST

PDB ID : 5T3W  
Title : Marburg virus VP30 bound to nucleoprotein  
Authors : Kirchdoerfer, R.K.; Moyer, C.L.; Abelson, D.M.; Saphire, E.O.  
Deposited on : 2016-08-26  
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

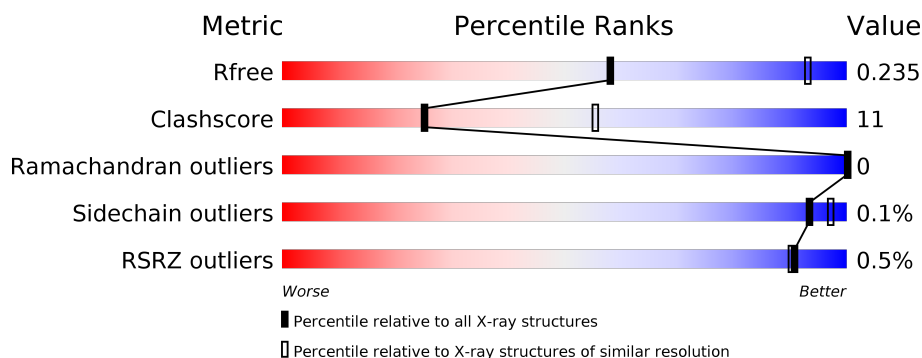
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	179	<div> <div>2%</div> <div>56%</div> <div>20%</div> <div>23%</div> </div>
1	B	179	<div> <div>58%</div> <div>18%</div> <div>23%</div> </div>
1	C	179	<div> <div>58%</div> <div>19%</div> <div>23%</div> </div>
1	D	179	<div> <div>63%</div> <div>13%</div> <div>23%</div> </div>
1	E	179	<div> <div>65%</div> <div>11%</div> <div>23%</div> </div>
1	F	179	<div> <div>2%</div> <div>58%</div> <div>18%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	179	 58% 19% 23%
1	H	179	 60% 16% 23%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8624 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 Fusion protein of Nucleoprotein and Minor nucleoprotein VP30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	B	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	C	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	D	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	E	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	F	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	G	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			
1	H	137	Total	C	N	O	S	0	0	0
			1078	683	186	204	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	initiating methionine	UNP P27588
A	104	ALA	-	expression tag	UNP P27588
A	105	HIS	-	expression tag	UNP P27588
A	106	HIS	-	expression tag	UNP P27588
A	107	HIS	-	expression tag	UNP P27588
A	108	HIS	-	expression tag	UNP P27588
A	109	HIS	-	expression tag	UNP P27588
A	110	HIS	-	expression tag	UNP P27588
A	111	VAL	-	expression tag	UNP P27588
A	112	ASP	-	expression tag	UNP P27588
A	113	ASP	-	expression tag	UNP P27588
A	114	ASP	-	expression tag	UNP P27588
A	115	ASP	-	expression tag	UNP P27588

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Chain	Residue	Modelled	Actual	Comment	Reference
A	116	LYS	-	expression tag	UNP P27588
A	117	MET	-	expression tag	UNP P27588
B	103	MET	-	initiating methionine	UNP P27588
B	104	ALA	-	expression tag	UNP P27588
B	105	HIS	-	expression tag	UNP P27588
B	106	HIS	-	expression tag	UNP P27588
B	107	HIS	-	expression tag	UNP P27588
B	108	HIS	-	expression tag	UNP P27588
B	109	HIS	-	expression tag	UNP P27588
B	110	HIS	-	expression tag	UNP P27588
B	111	VAL	-	expression tag	UNP P27588
B	112	ASP	-	expression tag	UNP P27588
B	113	ASP	-	expression tag	UNP P27588
B	114	ASP	-	expression tag	UNP P27588
B	115	ASP	-	expression tag	UNP P27588
B	116	LYS	-	expression tag	UNP P27588
B	117	MET	-	expression tag	UNP P27588
C	103	MET	-	initiating methionine	UNP P27588
C	104	ALA	-	expression tag	UNP P27588
C	105	HIS	-	expression tag	UNP P27588
C	106	HIS	-	expression tag	UNP P27588
C	107	HIS	-	expression tag	UNP P27588
C	108	HIS	-	expression tag	UNP P27588
C	109	HIS	-	expression tag	UNP P27588
C	110	HIS	-	expression tag	UNP P27588
C	111	VAL	-	expression tag	UNP P27588
C	112	ASP	-	expression tag	UNP P27588
C	113	ASP	-	expression tag	UNP P27588
C	114	ASP	-	expression tag	UNP P27588
C	115	ASP	-	expression tag	UNP P27588
C	116	LYS	-	expression tag	UNP P27588
C	117	MET	-	expression tag	UNP P27588
D	103	MET	-	initiating methionine	UNP P27588
D	104	ALA	-	expression tag	UNP P27588
D	105	HIS	-	expression tag	UNP P27588
D	106	HIS	-	expression tag	UNP P27588
D	107	HIS	-	expression tag	UNP P27588
D	108	HIS	-	expression tag	UNP P27588
D	109	HIS	-	expression tag	UNP P27588
D	110	HIS	-	expression tag	UNP P27588
D	111	VAL	-	expression tag	UNP P27588
D	112	ASP	-	expression tag	UNP P27588

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Chain	Residue	Modelled	Actual	Comment	Reference
D	113	ASP	-	expression tag	UNP P27588
D	114	ASP	-	expression tag	UNP P27588
D	115	ASP	-	expression tag	UNP P27588
D	116	LYS	-	expression tag	UNP P27588
D	117	MET	-	expression tag	UNP P27588
E	103	MET	-	initiating methionine	UNP P27588
E	104	ALA	-	expression tag	UNP P27588
E	105	HIS	-	expression tag	UNP P27588
E	106	HIS	-	expression tag	UNP P27588
E	107	HIS	-	expression tag	UNP P27588
E	108	HIS	-	expression tag	UNP P27588
E	109	HIS	-	expression tag	UNP P27588
E	110	HIS	-	expression tag	UNP P27588
E	111	VAL	-	expression tag	UNP P27588
E	112	ASP	-	expression tag	UNP P27588
E	113	ASP	-	expression tag	UNP P27588
E	114	ASP	-	expression tag	UNP P27588
E	115	ASP	-	expression tag	UNP P27588
E	116	LYS	-	expression tag	UNP P27588
E	117	MET	-	expression tag	UNP P27588
F	103	MET	-	initiating methionine	UNP P27588
F	104	ALA	-	expression tag	UNP P27588
F	105	HIS	-	expression tag	UNP P27588
F	106	HIS	-	expression tag	UNP P27588
F	107	HIS	-	expression tag	UNP P27588
F	108	HIS	-	expression tag	UNP P27588
F	109	HIS	-	expression tag	UNP P27588
F	110	HIS	-	expression tag	UNP P27588
F	111	VAL	-	expression tag	UNP P27588
F	112	ASP	-	expression tag	UNP P27588
F	113	ASP	-	expression tag	UNP P27588
F	114	ASP	-	expression tag	UNP P27588
F	115	ASP	-	expression tag	UNP P27588
F	116	LYS	-	expression tag	UNP P27588
F	117	MET	-	expression tag	UNP P27588
G	103	MET	-	initiating methionine	UNP P27588
G	104	ALA	-	expression tag	UNP P27588
G	105	HIS	-	expression tag	UNP P27588
G	106	HIS	-	expression tag	UNP P27588
G	107	HIS	-	expression tag	UNP P27588
G	108	HIS	-	expression tag	UNP P27588
G	109	HIS	-	expression tag	UNP P27588

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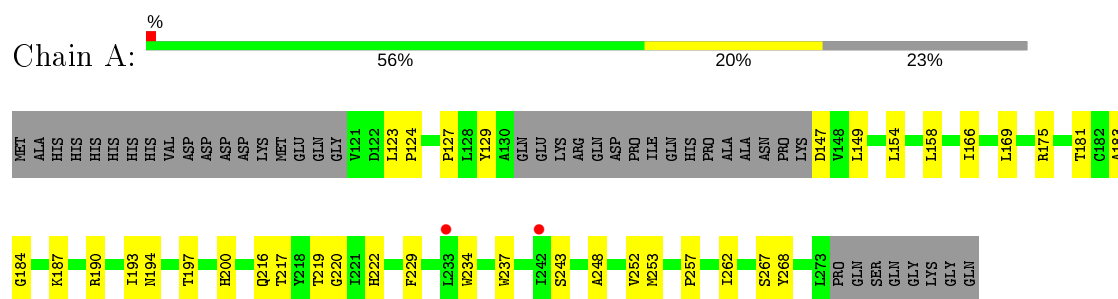
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Chain	Residue	Modelled	Actual	Comment	Reference
G	110	HIS	-	expression tag	UNP P27588
G	111	VAL	-	expression tag	UNP P27588
G	112	ASP	-	expression tag	UNP P27588
G	113	ASP	-	expression tag	UNP P27588
G	114	ASP	-	expression tag	UNP P27588
G	115	ASP	-	expression tag	UNP P27588
G	116	LYS	-	expression tag	UNP P27588
G	117	MET	-	expression tag	UNP P27588
H	103	MET	-	initiating methionine	UNP P27588
H	104	ALA	-	expression tag	UNP P27588
H	105	HIS	-	expression tag	UNP P27588
H	106	HIS	-	expression tag	UNP P27588
H	107	HIS	-	expression tag	UNP P27588
H	108	HIS	-	expression tag	UNP P27588
H	109	HIS	-	expression tag	UNP P27588
H	110	HIS	-	expression tag	UNP P27588
H	111	VAL	-	expression tag	UNP P27588
H	112	ASP	-	expression tag	UNP P27588
H	113	ASP	-	expression tag	UNP P27588
H	114	ASP	-	expression tag	UNP P27588
H	115	ASP	-	expression tag	UNP P27588
H	116	LYS	-	expression tag	UNP P27588
H	117	MET	-	expression tag	UNP P27588

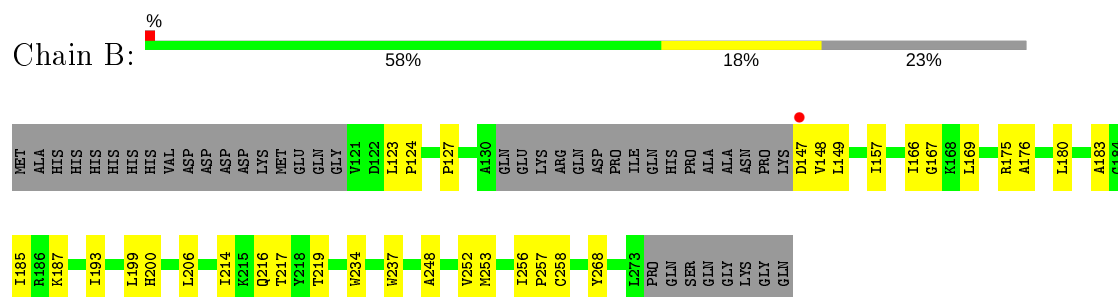
### 3 Residue-property plots [i](#)

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.

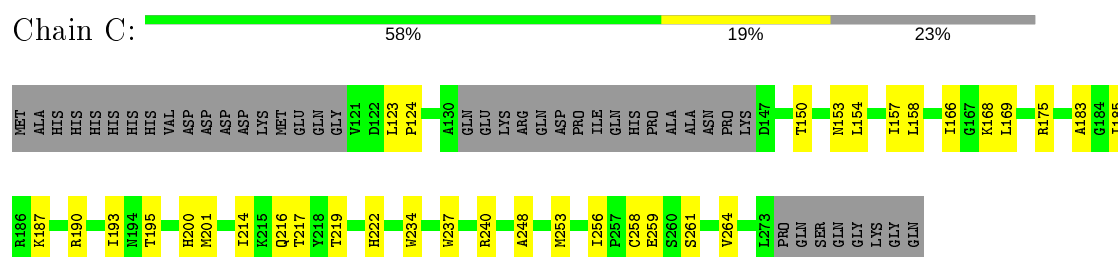
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



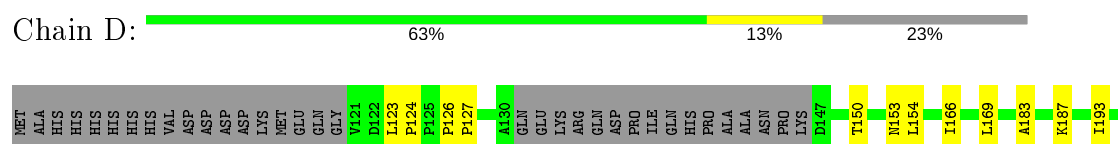
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



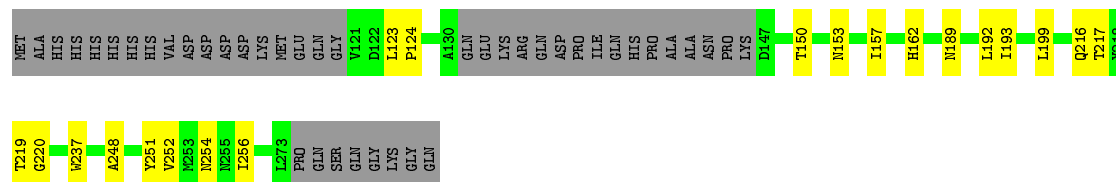
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



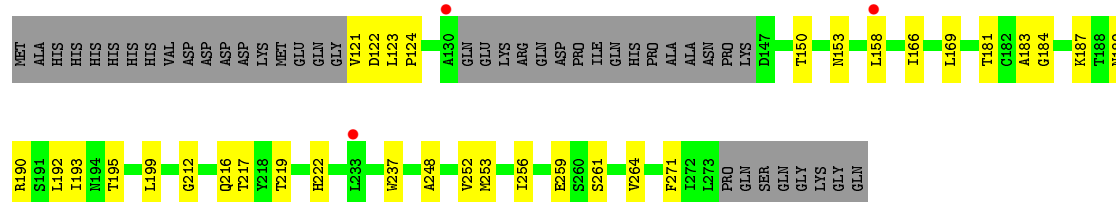




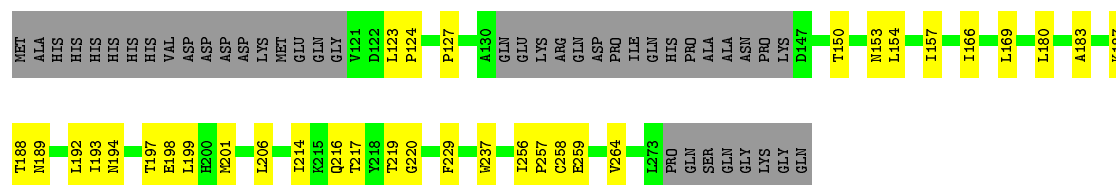
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



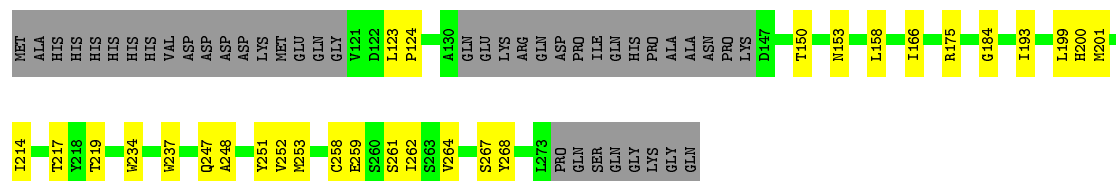
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.14Å 106.14Å 375.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	125.19 – 3.25 48.86 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (125.19-3.25) 100.0 (48.86-3.25)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.213 , 0.241 0.206 , 0.235	Depositor DCC
$R_{free}$ test set	1939 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	159.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 144.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	0.30	0/1100	0.49	0/1494
1	B	0.31	0/1100	0.55	1/1494 (0.1%)
1	C	0.31	0/1100	0.51	0/1494
1	D	0.31	0/1100	0.49	0/1494
1	E	0.31	0/1100	0.50	0/1494
1	F	0.35	0/1100	0.51	0/1494
1	G	0.30	0/1100	0.50	0/1494
1	H	0.32	0/1100	0.50	0/1494
All	All	0.31	0/8800	0.51	1/11952 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASP	CB-CG-OD2	5.25	123.02	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1078	0	1068	42	0
1	B	1078	0	1068	44	1
1	C	1078	0	1068	27	0
1	D	1078	0	1068	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1078	0	1068	16	0
1	F	1078	0	1068	25	0
1	G	1078	0	1068	30	0
1	H	1078	0	1068	30	1
All	All	8624	0	8544	184	1

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 11.

All (184) 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:A:267:SER:HB3	1:B:180:LEU:CD1	1.95	0.97
1:H:199:LEU:HD23	1:H:252:VAL:HG13	1.54	0.89
1:A:127:PRO:CG	1:B:214:ILE:HD11	2.11	0.81
1:F:212:GLY:O	1:F:216:GLN:HG2	1.81	0.79
1:A:267:SER:HB3	1:B:180:LEU:HD11	1.67	0.77
1:E:216:GLN:HB3	1:F:124:PRO:HG3	1.73	0.71
1:H:259:GLU:HG2	1:H:264:VAL:HG21	1.74	0.70
1:H:199:LEU:CD2	1:H:252:VAL:HA	2.22	0.70
1:H:199:LEU:HD23	1:H:252:VAL:HA	1.74	0.69
1:A:267:SER:CB	1:B:180:LEU:CD1	2.70	0.69
1:A:216:GLN:HB3	1:B:124:PRO:HG3	1.74	0.68
1:A:127:PRO:HG3	1:B:214:ILE:CD1	2.25	0.66
1:A:267:SER:CB	1:B:180:LEU:HD11	2.26	0.66
1:B:199:LEU:HD22	1:B:256:ILE:CD1	2.26	0.66
1:A:268:TYR:CD1	1:B:157:ILE:HG13	2.31	0.65
1:G:259:GLU:HG2	1:G:264:VAL:HG21	1.77	0.65
1:D:166:ILE:HA	1:D:169:LEU:HD13	1.79	0.64
1:A:268:TYR:HD1	1:B:157:ILE:HG13	1.63	0.64
1:C:193:ILE:HD13	1:C:219:THR:HG22	1.80	0.64
1:A:127:PRO:HG3	1:B:214:ILE:HD11	1.79	0.63
1:G:188:THR:HG22	1:G:258:CYS:HA	1.79	0.63
1:A:267:SER:HB3	1:B:180:LEU:HD13	1.79	0.63
1:B:148:VAL:HG12	1:B:149:LEU:N	2.12	0.62
1:G:166:ILE:HB	1:G:169:LEU:HD12	1.80	0.62
1:C:259:GLU:HG2	1:C:264:VAL:HG21	1.79	0.62
1:D:259:GLU:HG2	1:D:264:VAL:HG21	1.82	0.61
1:D:150:THR:HG23	1:D:153:ASN:H	1.66	0.61
1:A:217:THR:HG21	1:A:237:TRP:CZ2	2.34	0.61
1:A:124:PRO:HG3	1:B:216:GLN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ILE:HA	1:C:169:LEU:HD13	1.83	0.60
1:E:123:LEU:HD12	1:E:124:PRO:HD2	1.83	0.60
1:F:166:ILE:HA	1:F:169:LEU:HD13	1.83	0.60
1:A:127:PRO:HG2	1:B:214:ILE:HD11	1.84	0.59
1:C:217:THR:HG21	1:C:237:TRP:CZ2	2.38	0.59
1:A:149:LEU:O	1:B:257:PRO:HA	2.03	0.59
1:A:257:PRO:HG3	1:B:148:VAL:HG13	1.85	0.58
1:F:217:THR:HG21	1:F:237:TRP:CZ2	2.38	0.58
1:G:166:ILE:HA	1:G:169:LEU:HG	1.86	0.58
1:H:199:LEU:HD11	1:H:251:TYR:HE2	1.67	0.58
1:B:167:GLY:O	1:C:240:ARG:NH2	2.32	0.58
1:C:216:GLN:HB3	1:D:124:PRO:HG3	1.86	0.58
1:C:200:HIS:CE1	1:C:248:ALA:HB3	2.39	0.58
1:F:193:ILE:HG21	1:F:219:THR:HG23	1.86	0.57
1:H:193:ILE:HD13	1:H:219:THR:HG22	1.86	0.57
1:B:176:ALA:O	1:B:180:LEU:HD13	2.04	0.57
1:A:262:ILE:HD11	1:F:199:LEU:HD12	1.87	0.57
1:G:123:LEU:HD12	1:G:124:PRO:HD2	1.87	0.57
1:H:217:THR:HG21	1:H:237:TRP:CZ2	2.40	0.56
1:B:217:THR:HG21	1:B:237:TRP:CZ2	2.40	0.56
1:A:166:ILE:HD11	1:A:243:SER:O	2.05	0.56
1:H:150:THR:HG23	1:H:153:ASN:H	1.71	0.56
1:A:193:ILE:HG21	1:A:219:THR:HG23	1.89	0.55
1:H:199:LEU:HD23	1:H:252:VAL:CG1	2.31	0.55
1:G:150:THR:HG23	1:G:153:ASN:H	1.72	0.55
1:C:123:LEU:HD12	1:C:124:PRO:HD2	1.87	0.55
1:B:148:VAL:CG1	1:B:149:LEU:N	2.69	0.55
1:G:157:ILE:HD13	1:H:268:TYR:CD1	2.42	0.54
1:B:199:LEU:HD22	1:B:256:ILE:HD11	1.88	0.54
1:H:175:ARG:HD3	1:H:234:TRP:CD2	2.43	0.54
1:H:123:LEU:HD12	1:H:124:PRO:HD2	1.88	0.54
1:G:199:LEU:HD22	1:G:256:ILE:HD11	1.90	0.53
1:A:129:TYR:CZ	1:B:206:LEU:HD21	2.44	0.53
1:D:123:LEU:HD12	1:D:124:PRO:HD2	1.91	0.53
1:H:261:SER:HB3	1:H:264:VAL:HG22	1.91	0.53
1:C:154:LEU:O	1:C:157:ILE:HD12	2.09	0.53
1:A:129:TYR:CD2	1:C:168:LYS:HD3	2.44	0.53
1:A:194:ASN:HA	1:A:197:THR:HG22	1.90	0.53
1:F:261:SER:HB3	1:F:264:VAL:HG22	1.90	0.53
1:G:206:LEU:HD13	1:G:214:ILE:HD11	1.90	0.53
1:A:127:PRO:CG	1:B:214:ILE:CD1	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:GLU:HG2	1:F:264:VAL:HG21	1.90	0.52
1:E:217:THR:HG21	1:E:237:TRP:CZ2	2.44	0.52
1:F:195:THR:HG22	1:F:256:ILE:HD13	1.92	0.52
1:C:193:ILE:HG21	1:C:219:THR:HG23	1.91	0.51
1:H:166:ILE:HD11	1:H:247:GLN:N	2.25	0.51
1:F:189:ASN:HB2	1:F:192:LEU:HD12	1.93	0.51
1:A:262:ILE:CD1	1:F:199:LEU:HD12	2.41	0.51
1:G:166:ILE:HA	1:G:169:LEU:CD1	2.40	0.51
1:B:199:LEU:HD13	1:B:256:ILE:HD11	1.92	0.51
1:B:175:ARG:HD3	1:B:234:TRP:CD2	2.46	0.50
1:B:193:ILE:HD13	1:B:219:THR:HG22	1.93	0.50
1:D:193:ILE:HG21	1:D:219:THR:HG23	1.94	0.50
1:C:190:ARG:HG3	1:C:222:HIS:CE1	2.46	0.50
1:B:193:ILE:HG21	1:B:219:THR:HG23	1.93	0.50
1:A:127:PRO:HG3	1:B:214:ILE:HD13	1.94	0.49
1:H:199:LEU:HD11	1:H:251:TYR:CE2	2.47	0.49
1:G:166:ILE:HG22	1:G:169:LEU:HD11	1.93	0.49
1:H:193:ILE:HG21	1:H:219:THR:HG23	1.93	0.49
1:H:199:LEU:HD21	1:H:252:VAL:HA	1.95	0.49
1:F:190:ARG:HG3	1:F:222:HIS:CE1	2.48	0.49
1:F:193:ILE:HD13	1:F:219:THR:HG22	1.93	0.49
1:C:124:PRO:HG3	1:D:216:GLN:HB3	1.95	0.49
1:C:258:CYS:SG	1:D:154:LEU:HD12	2.53	0.48
1:G:183:ALA:O	1:G:187:LYS:HG2	2.13	0.48
1:A:147:ASP:O	1:B:268:TYR:HE2	1.97	0.48
1:G:154:LEU:HD12	1:H:258:CYS:SG	2.53	0.48
1:F:150:THR:HG23	1:F:153:ASN:H	1.78	0.48
1:D:248:ALA:O	1:D:252:VAL:HG23	2.14	0.48
1:C:150:THR:HG23	1:C:153:ASN:H	1.78	0.48
1:G:153:ASN:O	1:G:157:ILE:HG12	2.15	0.47
1:A:190:ARG:HG3	1:A:222:HIS:CE1	2.50	0.47
1:A:166:ILE:HA	1:A:169:LEU:HG	1.97	0.47
1:B:185:ILE:HG13	1:B:253:MET:HE1	1.97	0.47
1:D:217:THR:HG21	1:D:237:TRP:CZ2	2.50	0.47
1:G:157:ILE:HD12	1:G:180:LEU:HG	1.96	0.47
1:A:154:LEU:HD12	1:B:258:CYS:SG	2.54	0.47
1:C:261:SER:HB3	1:C:264:VAL:HG22	1.96	0.47
1:G:197:THR:O	1:G:201:MET:HG2	2.15	0.47
1:G:193:ILE:HD13	1:G:219:THR:HG22	1.96	0.47
1:E:193:ILE:HG21	1:E:219:THR:HG23	1.96	0.46
1:G:217:THR:HG21	1:G:237:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ILE:CB	1:G:169:LEU:HD12	2.45	0.46
1:G:193:ILE:HG21	1:G:219:THR:HG23	1.98	0.46
1:D:183:ALA:O	1:D:187:LYS:HG2	2.16	0.46
1:E:217:THR:HG23	1:F:124:PRO:HG2	1.98	0.46
1:G:157:ILE:HD13	1:H:268:TYR:HD1	1.80	0.46
1:G:216:GLN:HB3	1:H:124:PRO:HG3	1.98	0.45
1:A:237:TRP:CH2	1:B:127:PRO:HD3	2.51	0.45
1:E:189:ASN:HB2	1:E:192:LEU:HD12	1.97	0.45
1:D:261:SER:HB3	1:D:264:VAL:HG22	1.97	0.45
1:B:200:HIS:CE1	1:B:248:ALA:HB3	2.52	0.45
1:E:193:ILE:HD13	1:E:219:THR:HG22	1.97	0.45
1:C:157:ILE:HD12	1:C:158:LEU:N	2.31	0.45
1:C:201:MET:SD	1:C:214:ILE:HD13	2.56	0.45
1:F:248:ALA:O	1:F:252:VAL:HG23	2.16	0.45
1:H:248:ALA:O	1:H:252:VAL:HG23	2.17	0.45
1:B:157:ILE:HG21	1:B:180:LEU:CD2	2.47	0.44
1:B:183:ALA:O	1:B:187:LYS:HG2	2.17	0.44
1:G:189:ASN:HB2	1:G:192:LEU:HD12	2.00	0.44
1:F:183:ALA:O	1:F:187:LYS:HG2	2.17	0.44
1:F:121:VAL:HG12	1:F:122:ASP:H	1.83	0.44
1:F:123:LEU:HD12	1:F:124:PRO:HD2	1.98	0.44
1:E:199:LEU:HD22	1:E:251:TYR:HE2	1.83	0.44
1:G:127:PRO:HD3	1:H:237:TRP:CH2	2.53	0.44
1:H:199:LEU:HD23	1:H:252:VAL:CA	2.46	0.44
1:A:183:ALA:O	1:A:187:LYS:HG2	2.18	0.43
1:E:162:HIS:CE1	1:E:254:ASN:HD22	2.35	0.43
1:A:175:ARG:HD3	1:A:234:TRP:CD2	2.53	0.43
1:A:248:ALA:O	1:A:252:VAL:HG23	2.18	0.43
1:E:248:ALA:O	1:E:252:VAL:HG23	2.18	0.43
1:C:259:GLU:HG2	1:C:264:VAL:CG2	2.47	0.43
1:F:252:VAL:HG13	1:F:256:ILE:HD12	2.00	0.43
1:A:124:PRO:HG2	1:B:217:THR:HG23	2.00	0.43
1:B:248:ALA:O	1:B:252:VAL:HG23	2.19	0.43
1:C:195:THR:HG22	1:C:256:ILE:HD13	2.00	0.43
1:E:124:PRO:HG3	1:F:216:GLN:HB2	1.99	0.43
1:B:256:ILE:HG23	1:B:257:PRO:HD2	2.01	0.42
1:C:185:ILE:HG13	1:C:253:MET:HE1	2.01	0.42
1:H:158:LEU:HD11	1:H:184:GLY:HA3	2.00	0.42
1:E:150:THR:HG23	1:E:153:ASN:H	1.85	0.42
1:B:166:ILE:HA	1:B:169:LEU:HG	2.01	0.42
1:C:183:ALA:O	1:C:187:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD12	1:B:124:PRO:HD2	2.01	0.42
1:E:220:GLY:HA2	1:F:121:VAL:HG11	2.02	0.42
1:H:200:HIS:CE1	1:H:248:ALA:HB3	2.55	0.42
1:A:129:TYR:CE2	1:B:206:LEU:HD21	2.55	0.42
1:A:194:ASN:O	1:A:197:THR:HG22	2.20	0.42
1:F:181:THR:HG23	1:F:253:MET:HE1	2.02	0.41
1:F:158:LEU:HD11	1:F:184:GLY:HA3	2.02	0.41
1:E:199:LEU:CD2	1:E:251:TYR:HE2	2.31	0.41
1:A:181:THR:HG23	1:A:253:MET:HE1	2.02	0.41
1:E:252:VAL:HG13	1:E:256:ILE:HD12	2.01	0.41
1:D:201:MET:SD	1:D:214:ILE:HD13	2.61	0.41
1:G:256:ILE:HG23	1:G:257:PRO:HD2	2.01	0.41
1:B:157:ILE:HG21	1:B:180:LEU:HD23	2.01	0.41
1:G:180:LEU:HD13	1:H:267:SER:HB3	2.02	0.41
1:A:200:HIS:CE1	1:A:248:ALA:HB3	2.55	0.41
1:C:217:THR:HG23	1:D:124:PRO:HG2	2.02	0.41
1:C:214:ILE:HD11	1:D:127:PRO:HB3	2.01	0.41
1:A:257:PRO:HG3	1:B:148:VAL:CG1	2.50	0.41
1:G:217:THR:HG23	1:H:124:PRO:HG2	2.02	0.41
1:C:175:ARG:HD3	1:C:234:TRP:CD2	2.56	0.41
1:G:166:ILE:HA	1:G:169:LEU:CG	2.51	0.41
1:A:158:LEU:HD11	1:A:184:GLY:HA3	2.03	0.40
1:A:220:GLY:HA3	1:A:229:PHE:CE2	2.56	0.40
1:H:201:MET:SD	1:H:214:ILE:HD13	2.61	0.40
1:C:154:LEU:HD12	1:D:258:CYS:SG	2.62	0.40
1:E:157:ILE:HD11	1:F:271:PHE:HB2	2.03	0.40
1:G:220:GLY:HA3	1:G:229:PHE:CE2	2.56	0.40
1:H:259:GLU:HG2	1:H:264:VAL:CG2	2.46	0.40
1:A:123:LEU:HD12	1:A:124:PRO:HD2	2.03	0.40
1:G:194:ASN:O	1:G:198:GLU:HB2	2.20	0.40
1:C:237:TRP:CZ2	1:D:126:PRO:HA	2.57	0.40
1:H:150:THR:HG22	1:H:153:ASN:ND2	2.36	0.40

All (1) 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:B:199:LEU:CD1	1:H:262:ILE:CD1[4_545]	2.00	0.20



## 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	133/179 (74%)	130 (98%)	3 (2%)	0	100	100
1	B	133/179 (74%)	131 (98%)	2 (2%)	0	100	100
1	C	133/179 (74%)	129 (97%)	4 (3%)	0	100	100
1	D	133/179 (74%)	130 (98%)	3 (2%)	0	100	100
1	E	133/179 (74%)	130 (98%)	3 (2%)	0	100	100
1	F	133/179 (74%)	129 (97%)	4 (3%)	0	100	100
1	G	133/179 (74%)	129 (97%)	4 (3%)	0	100	100
1	H	133/179 (74%)	130 (98%)	3 (2%)	0	100	100
All	All	1064/1432 (74%)	1038 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	120/156 (77%)	120 (100%)	0	100	100
1	B	120/156 (77%)	120 (100%)	0	100	100
1	C	120/156 (77%)	120 (100%)	0	100	100
1	D	120/156 (77%)	120 (100%)	0	100	100
1	E	120/156 (77%)	120 (100%)	0	100	100
1	F	120/156 (77%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	120/156 (77%)	120 (100%)	0	100	100
1	H	120/156 (77%)	119 (99%)	1 (1%)	81	89
All	All	960/1248 (77%)	959 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	253	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	137/179 (76%)	0.08	2 (1%) 73 71	120, 144, 177, 198	0
1	B	137/179 (76%)	-0.00	1 (0%) 87 88	94, 140, 173, 197	0
1	C	137/179 (76%)	-0.08	0 100 100	117, 138, 173, 187	0
1	D	137/179 (76%)	0.06	0 100 100	123, 143, 173, 183	0
1	E	137/179 (76%)	0.01	0 100 100	117, 143, 177, 203	0
1	F	137/179 (76%)	0.17	3 (2%) 62 59	128, 150, 180, 189	0
1	G	137/179 (76%)	0.07	0 100 100	125, 145, 175, 189	0
1	H	137/179 (76%)	-0.05	0 100 100	117, 140, 170, 200	0
All	All	1096/1432 (76%)	0.03	6 (0%) 91 90	94, 143, 176, 203	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ASP	3.7
1	F	233	LEU	2.5
1	F	130	ALA	2.5
1	A	233	LEU	2.2
1	A	242	ILE	2.1
1	F	158	LEU	2.1

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.