



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:23 PM UTC

PDB ID : 3BP9 / pdb_00003bp9
Title : Structure of B-tropic MLV capsid N-terminal domain
Authors : Gulnagar, M.B.; Dodding, M.P.; Goldstone, D.C.; Haire, L.F.; Stoye, J.P.;
Taylor, I.A.
Deposited on : 2007-12-18
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

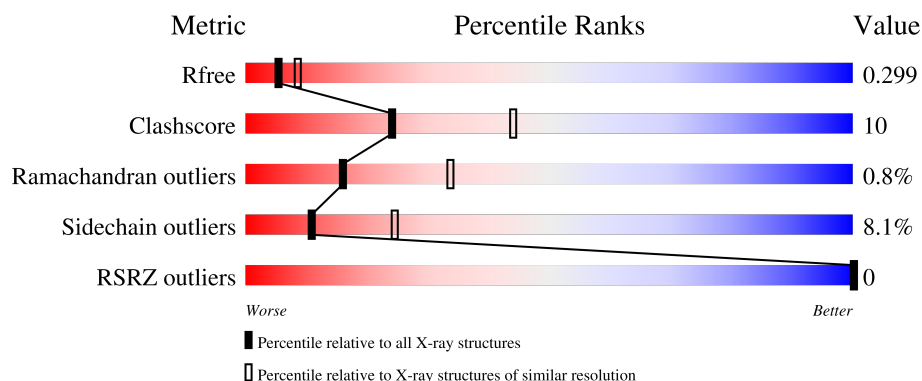
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



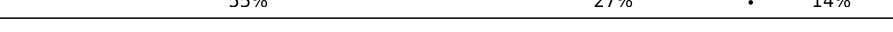
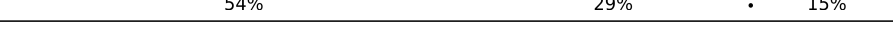
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	140	 70% 20% • 6%
1	B	140	 74% 14% • 10%
1	C	140	 70% 22% • 6%
1	D	140	 79% 14% • 6%
1	E	140	 78% 14% • 6%

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Mol	Chain	Length	Quality of chain
1	F	140	 80% 14% 6%
1	G	140	 59% 30% 7%
1	H	140	 73% 15% 9%
1	I	140	 74% 16% 6%
1	J	140	 77% 17% 6%
1	K	140	 75% 16% 6%
1	L	140	 81% 13% 6%
1	M	140	 74% 18% 6%
1	N	140	 66% 24% 9%
1	O	140	 55% 27% 16%
1	P	140	 56% 27% 14%
1	Q	140	 60% 26% 11%
1	R	140	 57% 28% 12%
1	S	140	 80% 11% 6%
1	T	140	 66% 26% 6%
1	U	140	 55% 27% 14%
1	V	140	 54% 29% 15%
1	X	140	 68% 19% 11%
1	Y	140	 59% 26% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24586 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 Gag protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			1033	648	184	200	1			
1	B	126	Total	C	N	O	S	0	0	0
			1008	635	178	194	1			
1	C	131	Total	C	N	O	S	0	1	0
			1051	659	189	202	1			
1	D	131	Total	C	N	O	S	0	0	0
			1032	649	183	199	1			
1	E	132	Total	C	N	O	S	0	1	0
			1053	665	186	201	1			
1	F	131	Total	C	N	O	S	0	0	0
			1040	653	185	201	1			
1	G	130	Total	C	N	O	S	0	0	0
			1022	641	182	198	1			
1	H	128	Total	C	N	O	S	0	0	0
			1017	640	180	196	1			
1	I	131	Total	C	N	O	S	0	0	0
			1042	654	187	200	1			
1	J	132	Total	C	N	O	S	0	1	0
			1055	662	191	201	1			
1	K	131	Total	C	N	O	S	0	1	0
			1050	662	186	201	1			
1	L	131	Total	C	N	O	S	0	1	0
			1040	654	183	202	1			
1	M	132	Total	C	N	O	S	0	0	0
			1030	647	180	202	1			
1	N	128	Total	C	N	O	S	0	0	0
			1009	638	175	195	1			
1	O	118	Total	C	N	O	S	0	0	0
			941	597	162	181	1			
1	P	121	Total	C	N	O	S	0	0	0
			937	594	161	181	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	125	Total 983	C 621	N 171	O 190	S 1	0	0	0
1	R	123	Total 957	C 604	N 165	O 187	S 1	0	0	0
1	S	132	Total 1039	C 653	N 183	O 202	S 1	0	0	0
1	T	132	Total 1045	C 656	N 186	O 202	S 1	0	0	0
1	U	120	Total 959	C 606	N 168	O 184	S 1	0	0	0
1	V	119	Total 929	C 591	N 163	O 174	S 1	0	0	0
1	X	124	Total 986	C 624	N 171	O 190	S 1	0	0	0
1	Y	124	Total 983	C 621	N 170	O 191	S 1	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	-	expression tag	UNP Q9WHV6
A	134	GLU	-	expression tag	UNP Q9WHV6
A	135	HIS	-	expression tag	UNP Q9WHV6
A	136	HIS	-	expression tag	UNP Q9WHV6
A	137	HIS	-	expression tag	UNP Q9WHV6
A	138	HIS	-	expression tag	UNP Q9WHV6
A	139	HIS	-	expression tag	UNP Q9WHV6
A	140	HIS	-	expression tag	UNP Q9WHV6
B	133	LEU	-	expression tag	UNP Q9WHV6
B	134	GLU	-	expression tag	UNP Q9WHV6
B	135	HIS	-	expression tag	UNP Q9WHV6
B	136	HIS	-	expression tag	UNP Q9WHV6
B	137	HIS	-	expression tag	UNP Q9WHV6
B	138	HIS	-	expression tag	UNP Q9WHV6
B	139	HIS	-	expression tag	UNP Q9WHV6
B	140	HIS	-	expression tag	UNP Q9WHV6
C	133	LEU	-	expression tag	UNP Q9WHV6
C	134	GLU	-	expression tag	UNP Q9WHV6
C	135	HIS	-	expression tag	UNP Q9WHV6
C	136	HIS	-	expression tag	UNP Q9WHV6
C	137	HIS	-	expression tag	UNP Q9WHV6
C	138	HIS	-	expression tag	UNP Q9WHV6
C	139	HIS	-	expression tag	UNP Q9WHV6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	140	HIS	-	expression tag	UNP Q9WHV6
D	133	LEU	-	expression tag	UNP Q9WHV6
D	134	GLU	-	expression tag	UNP Q9WHV6
D	135	HIS	-	expression tag	UNP Q9WHV6
D	136	HIS	-	expression tag	UNP Q9WHV6
D	137	HIS	-	expression tag	UNP Q9WHV6
D	138	HIS	-	expression tag	UNP Q9WHV6
D	139	HIS	-	expression tag	UNP Q9WHV6
D	140	HIS	-	expression tag	UNP Q9WHV6
E	133	LEU	-	expression tag	UNP Q9WHV6
E	134	GLU	-	expression tag	UNP Q9WHV6
E	135	HIS	-	expression tag	UNP Q9WHV6
E	136	HIS	-	expression tag	UNP Q9WHV6
E	137	HIS	-	expression tag	UNP Q9WHV6
E	138	HIS	-	expression tag	UNP Q9WHV6
E	139	HIS	-	expression tag	UNP Q9WHV6
E	140	HIS	-	expression tag	UNP Q9WHV6
F	133	LEU	-	expression tag	UNP Q9WHV6
F	134	GLU	-	expression tag	UNP Q9WHV6
F	135	HIS	-	expression tag	UNP Q9WHV6
F	136	HIS	-	expression tag	UNP Q9WHV6
F	137	HIS	-	expression tag	UNP Q9WHV6
F	138	HIS	-	expression tag	UNP Q9WHV6
F	139	HIS	-	expression tag	UNP Q9WHV6
F	140	HIS	-	expression tag	UNP Q9WHV6
G	133	LEU	-	expression tag	UNP Q9WHV6
G	134	GLU	-	expression tag	UNP Q9WHV6
G	135	HIS	-	expression tag	UNP Q9WHV6
G	136	HIS	-	expression tag	UNP Q9WHV6
G	137	HIS	-	expression tag	UNP Q9WHV6
G	138	HIS	-	expression tag	UNP Q9WHV6
G	139	HIS	-	expression tag	UNP Q9WHV6
G	140	HIS	-	expression tag	UNP Q9WHV6
H	133	LEU	-	expression tag	UNP Q9WHV6
H	134	GLU	-	expression tag	UNP Q9WHV6
H	135	HIS	-	expression tag	UNP Q9WHV6
H	136	HIS	-	expression tag	UNP Q9WHV6
H	137	HIS	-	expression tag	UNP Q9WHV6
H	138	HIS	-	expression tag	UNP Q9WHV6
H	139	HIS	-	expression tag	UNP Q9WHV6
H	140	HIS	-	expression tag	UNP Q9WHV6
I	133	LEU	-	expression tag	UNP Q9WHV6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	134	GLU	-	expression tag	UNP Q9WHV6
I	135	HIS	-	expression tag	UNP Q9WHV6
I	136	HIS	-	expression tag	UNP Q9WHV6
I	137	HIS	-	expression tag	UNP Q9WHV6
I	138	HIS	-	expression tag	UNP Q9WHV6
I	139	HIS	-	expression tag	UNP Q9WHV6
I	140	HIS	-	expression tag	UNP Q9WHV6
J	133	LEU	-	expression tag	UNP Q9WHV6
J	134	GLU	-	expression tag	UNP Q9WHV6
J	135	HIS	-	expression tag	UNP Q9WHV6
J	136	HIS	-	expression tag	UNP Q9WHV6
J	137	HIS	-	expression tag	UNP Q9WHV6
J	138	HIS	-	expression tag	UNP Q9WHV6
J	139	HIS	-	expression tag	UNP Q9WHV6
J	140	HIS	-	expression tag	UNP Q9WHV6
K	133	LEU	-	expression tag	UNP Q9WHV6
K	134	GLU	-	expression tag	UNP Q9WHV6
K	135	HIS	-	expression tag	UNP Q9WHV6
K	136	HIS	-	expression tag	UNP Q9WHV6
K	137	HIS	-	expression tag	UNP Q9WHV6
K	138	HIS	-	expression tag	UNP Q9WHV6
K	139	HIS	-	expression tag	UNP Q9WHV6
K	140	HIS	-	expression tag	UNP Q9WHV6
L	133	LEU	-	expression tag	UNP Q9WHV6
L	134	GLU	-	expression tag	UNP Q9WHV6
L	135	HIS	-	expression tag	UNP Q9WHV6
L	136	HIS	-	expression tag	UNP Q9WHV6
L	137	HIS	-	expression tag	UNP Q9WHV6
L	138	HIS	-	expression tag	UNP Q9WHV6
L	139	HIS	-	expression tag	UNP Q9WHV6
L	140	HIS	-	expression tag	UNP Q9WHV6
M	133	LEU	-	expression tag	UNP Q9WHV6
M	134	GLU	-	expression tag	UNP Q9WHV6
M	135	HIS	-	expression tag	UNP Q9WHV6
M	136	HIS	-	expression tag	UNP Q9WHV6
M	137	HIS	-	expression tag	UNP Q9WHV6
M	138	HIS	-	expression tag	UNP Q9WHV6
M	139	HIS	-	expression tag	UNP Q9WHV6
M	140	HIS	-	expression tag	UNP Q9WHV6
N	133	LEU	-	expression tag	UNP Q9WHV6
N	134	GLU	-	expression tag	UNP Q9WHV6
N	135	HIS	-	expression tag	UNP Q9WHV6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	136	HIS	-	expression tag	UNP Q9WHV6
N	137	HIS	-	expression tag	UNP Q9WHV6
N	138	HIS	-	expression tag	UNP Q9WHV6
N	139	HIS	-	expression tag	UNP Q9WHV6
N	140	HIS	-	expression tag	UNP Q9WHV6
O	133	LEU	-	expression tag	UNP Q9WHV6
O	134	GLU	-	expression tag	UNP Q9WHV6
O	135	HIS	-	expression tag	UNP Q9WHV6
O	136	HIS	-	expression tag	UNP Q9WHV6
O	137	HIS	-	expression tag	UNP Q9WHV6
O	138	HIS	-	expression tag	UNP Q9WHV6
O	139	HIS	-	expression tag	UNP Q9WHV6
O	140	HIS	-	expression tag	UNP Q9WHV6
P	133	LEU	-	expression tag	UNP Q9WHV6
P	134	GLU	-	expression tag	UNP Q9WHV6
P	135	HIS	-	expression tag	UNP Q9WHV6
P	136	HIS	-	expression tag	UNP Q9WHV6
P	137	HIS	-	expression tag	UNP Q9WHV6
P	138	HIS	-	expression tag	UNP Q9WHV6
P	139	HIS	-	expression tag	UNP Q9WHV6
P	140	HIS	-	expression tag	UNP Q9WHV6
Q	133	LEU	-	expression tag	UNP Q9WHV6
Q	134	GLU	-	expression tag	UNP Q9WHV6
Q	135	HIS	-	expression tag	UNP Q9WHV6
Q	136	HIS	-	expression tag	UNP Q9WHV6
Q	137	HIS	-	expression tag	UNP Q9WHV6
Q	138	HIS	-	expression tag	UNP Q9WHV6
Q	139	HIS	-	expression tag	UNP Q9WHV6
Q	140	HIS	-	expression tag	UNP Q9WHV6
R	133	LEU	-	expression tag	UNP Q9WHV6
R	134	GLU	-	expression tag	UNP Q9WHV6
R	135	HIS	-	expression tag	UNP Q9WHV6
R	136	HIS	-	expression tag	UNP Q9WHV6
R	137	HIS	-	expression tag	UNP Q9WHV6
R	138	HIS	-	expression tag	UNP Q9WHV6
R	139	HIS	-	expression tag	UNP Q9WHV6
R	140	HIS	-	expression tag	UNP Q9WHV6
S	133	LEU	-	expression tag	UNP Q9WHV6
S	134	GLU	-	expression tag	UNP Q9WHV6
S	135	HIS	-	expression tag	UNP Q9WHV6
S	136	HIS	-	expression tag	UNP Q9WHV6
S	137	HIS	-	expression tag	UNP Q9WHV6

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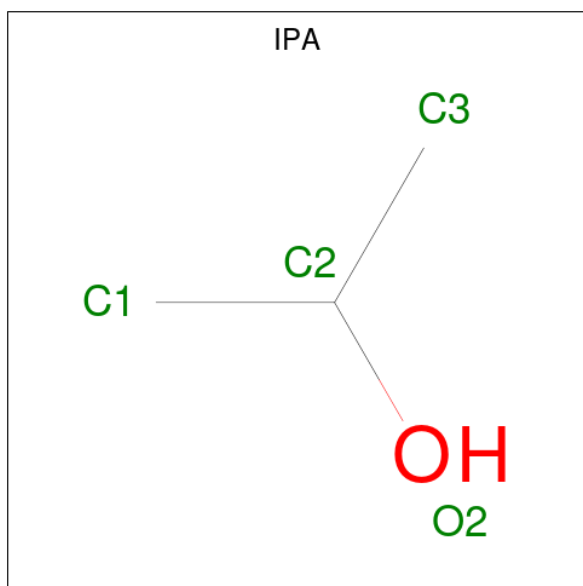
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S	139	HIS	-	expression tag	UNP Q9WHV6
S	140	HIS	-	expression tag	UNP Q9WHV6
T	133	LEU	-	expression tag	UNP Q9WHV6
T	134	GLU	-	expression tag	UNP Q9WHV6
T	135	HIS	-	expression tag	UNP Q9WHV6
T	136	HIS	-	expression tag	UNP Q9WHV6
T	137	HIS	-	expression tag	UNP Q9WHV6
T	138	HIS	-	expression tag	UNP Q9WHV6
T	139	HIS	-	expression tag	UNP Q9WHV6
T	140	HIS	-	expression tag	UNP Q9WHV6
U	133	LEU	-	expression tag	UNP Q9WHV6
U	134	GLU	-	expression tag	UNP Q9WHV6
U	135	HIS	-	expression tag	UNP Q9WHV6
U	136	HIS	-	expression tag	UNP Q9WHV6
U	137	HIS	-	expression tag	UNP Q9WHV6
U	138	HIS	-	expression tag	UNP Q9WHV6
U	139	HIS	-	expression tag	UNP Q9WHV6
U	140	HIS	-	expression tag	UNP Q9WHV6
V	133	LEU	-	expression tag	UNP Q9WHV6
V	134	GLU	-	expression tag	UNP Q9WHV6
V	135	HIS	-	expression tag	UNP Q9WHV6
V	136	HIS	-	expression tag	UNP Q9WHV6
V	137	HIS	-	expression tag	UNP Q9WHV6
V	138	HIS	-	expression tag	UNP Q9WHV6
V	139	HIS	-	expression tag	UNP Q9WHV6
V	140	HIS	-	expression tag	UNP Q9WHV6
X	133	LEU	-	expression tag	UNP Q9WHV6
X	134	GLU	-	expression tag	UNP Q9WHV6
X	135	HIS	-	expression tag	UNP Q9WHV6
X	136	HIS	-	expression tag	UNP Q9WHV6
X	137	HIS	-	expression tag	UNP Q9WHV6
X	138	HIS	-	expression tag	UNP Q9WHV6
X	139	HIS	-	expression tag	UNP Q9WHV6
X	140	HIS	-	expression tag	UNP Q9WHV6
Y	133	LEU	-	expression tag	UNP Q9WHV6
Y	134	GLU	-	expression tag	UNP Q9WHV6
Y	135	HIS	-	expression tag	UNP Q9WHV6
Y	136	HIS	-	expression tag	UNP Q9WHV6
Y	137	HIS	-	expression tag	UNP Q9WHV6
Y	138	HIS	-	expression tag	UNP Q9WHV6
Y	139	HIS	-	expression tag	UNP Q9WHV6

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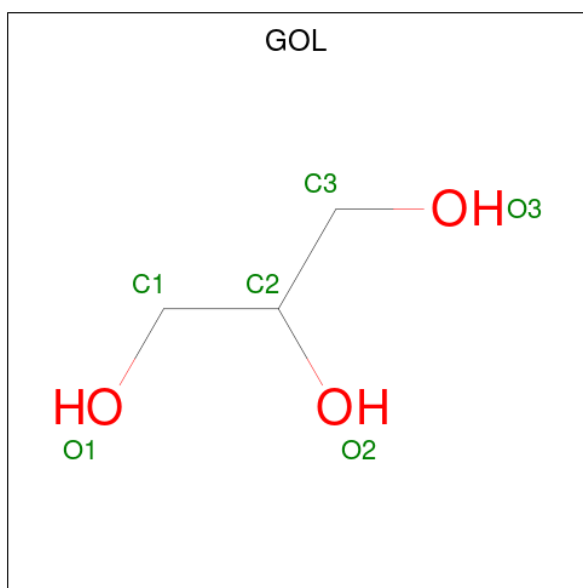
Chain	Residue	Modelled	Actual	Comment	Reference
Y	140	HIS	-	expression tag	UNP Q9WHV6

- Molecule 2 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	3	1		
2	C	1	Total	C	O	0	0
			4	3	1		
2	D	1	Total	C	O	0	0
			4	3	1		
2	E	1	Total	C	O	0	0
			4	3	1		
2	E	1	Total	C	O	0	0
			4	3	1		
2	F	1	Total	C	O	0	0
			4	3	1		
2	G	1	Total	C	O	0	0
			4	3	1		
2	I	1	Total	C	O	0	0
			4	3	1		
2	J	1	Total	C	O	0	0
			4	3	1		
2	K	1	Total	C	O	0	0
			4	3	1		
2	K	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	16	Total	O	0	0
			16	16		
4	C	12	Total	O	0	0
			12	12		
4	D	23	Total	O	0	0
			23	23		
4	E	17	Total	O	0	0
			17	17		
4	F	17	Total	O	0	0
			17	17		
4	G	12	Total	O	0	0
			12	12		
4	H	20	Total	O	0	0
			20	20		
4	I	16	Total	O	0	0
			16	16		

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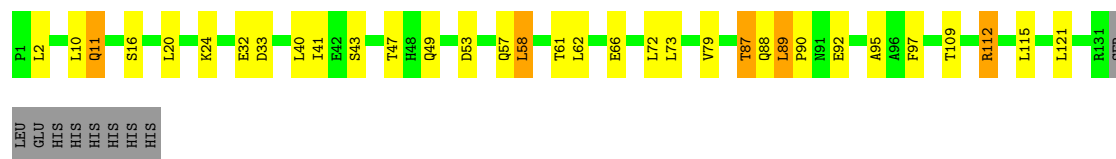
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	27	Total 27	O 27	0	0
4	K	13	Total 13	O 13	0	0
4	L	25	Total 25	O 25	0	0
4	M	9	Total 9	O 9	0	0
4	N	9	Total 9	O 9	0	0
4	O	1	Total 1	O 1	0	0
4	P	6	Total 6	O 6	0	0
4	Q	7	Total 7	O 7	0	0
4	R	6	Total 6	O 6	0	0
4	S	5	Total 5	O 5	0	0
4	T	4	Total 4	O 4	0	0
4	U	3	Total 3	O 3	0	0
4	V	7	Total 7	O 7	0	0
4	X	6	Total 6	O 6	0	0
4	Y	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Gag protein

Chain A: 



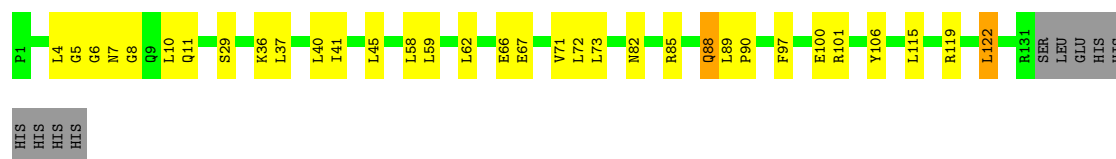
- Molecule 1: Gag protein

Chain B: 



- Molecule 1: Gag protein

Chain C: 



- Molecule 1: Gag protein

Chain D: 



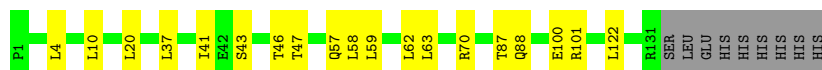
- Molecule 1: Gag protein

Chain E: 



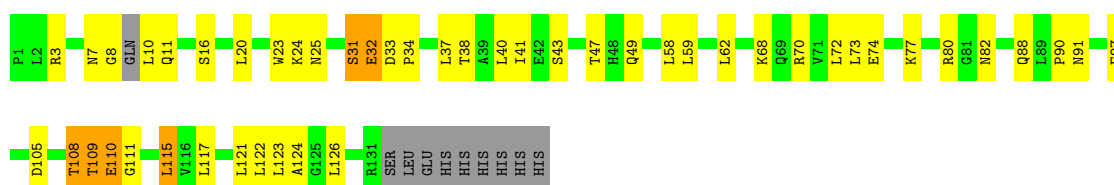
- Molecule 1: Gag protein

Chain F: 80% 14% 6%



- Molecule 1: Gag protein

Chain G: 59% 30% 7%



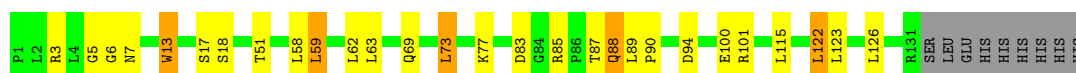
- Molecule 1: Gag protein

Chain H: 73% 15% 9%



- Molecule 1: Gag protein

Chain I: 74% 16% 6%



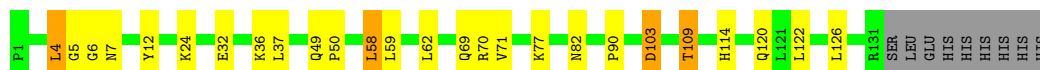
- Molecule 1: Gag protein

Chain J: 77% 17% 6%



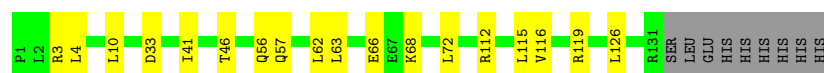
- Molecule 1: Gag protein

Chain K: 75% 16% 6%



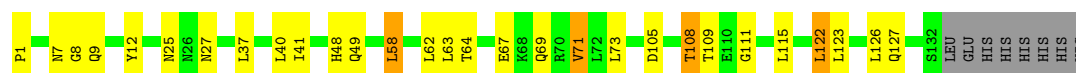
- Molecule 1: Gag protein

Chain L:  81% 13% 6%



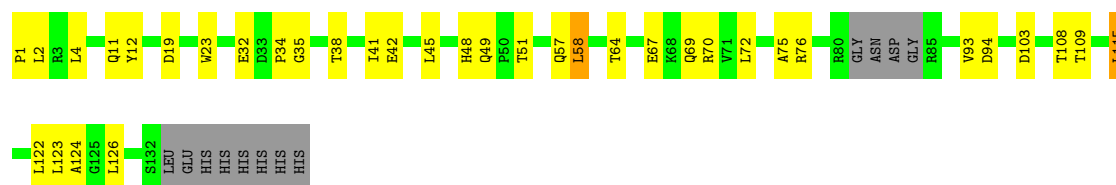
• Molecule 1: Gag protein

Chain M:  74% 18% 6%



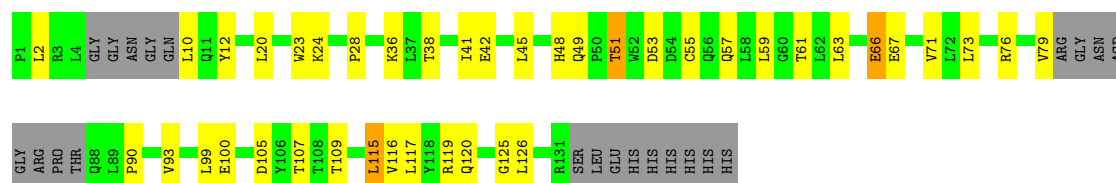
• Molecule 1: Gag protein

Chain N:  66% 24% 9%



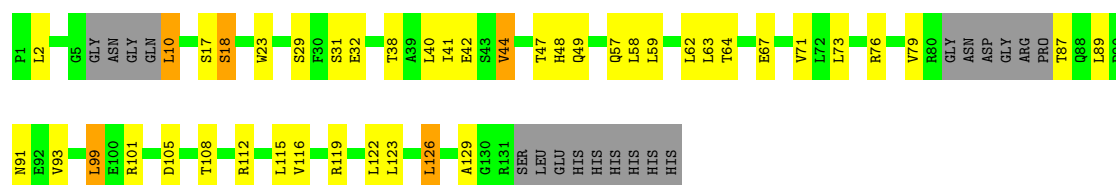
• Molecule 1: Gag protein

Chain O:  55% 27% 16%



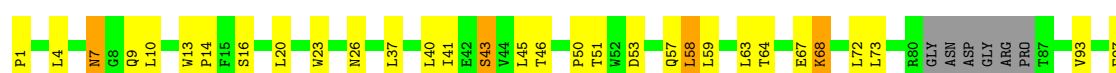
• Molecule 1: Gag protein

Chain P:  56% 27% 14%



• Molecule 1: Gag protein

Chain Q:  60% 26% 11%

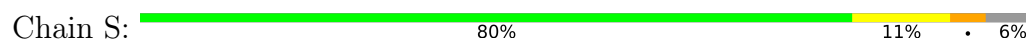




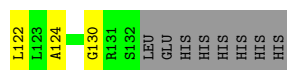
• Molecule 1: Gag protein



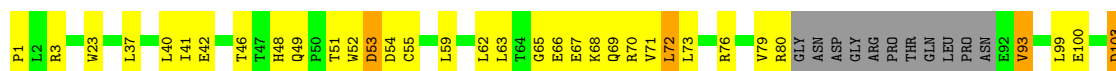
• Molecule 1: Gag protein



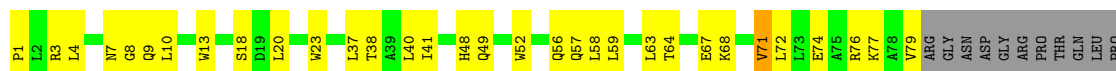
• Molecule 1: Gag protein



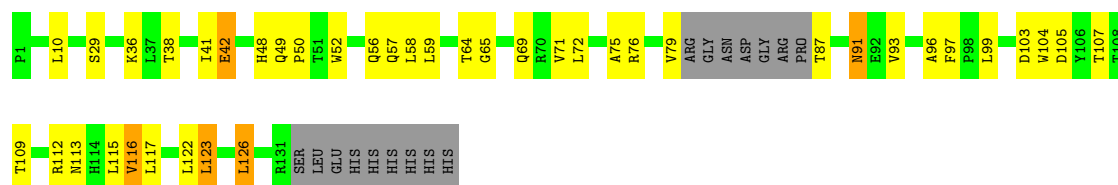
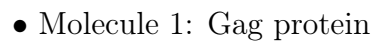
• Molecule 1: Gag protein



• Molecule 1: Gag protein



Chain X: 68% 19% • 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.26Å 86.83Å 152.36Å 89.12° 90.04° 60.26°	Depositor
Resolution (Å)	17.16 – 2.60 17.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (17.16-2.60) 96.6 (17.16-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.292 0.229 , 0.299	Depositor DCC
R_{free} test set	5709 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for h-k,h,l 0.029 for k,-h+k,l 0.013 for -k,h-k,l 0.013 for -h+k,-h,l 0.477 for h,h-k,-l 0.014 for -h+k,k,-l 0.018 for -h,-k,l 0.014 for -k,-h,-l 0.032 for k,h,-l 0.017 for -h,-h+k,-l 0.029 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24586	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IPA

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	0.94	0/1058	0.99	0/1443
1	B	0.98	0/1032	1.01	1/1407 (0.1%)
1	C	1.01	0/1079	1.01	0/1470
1	D	0.98	0/1057	0.94	0/1442
1	E	0.95	1/1083 (0.1%)	0.96	0/1479
1	F	0.95	0/1065	0.97	0/1452
1	G	0.94	0/1046	1.03	2/1425 (0.1%)
1	H	0.98	0/1041	0.98	1/1419 (0.1%)
1	I	0.96	0/1067	1.02	1/1454 (0.1%)
1	J	0.94	0/1083	0.99	0/1475
1	K	0.95	0/1077	1.02	0/1471
1	L	0.96	1/1068 (0.1%)	1.00	3/1457 (0.2%)
1	M	0.81	0/1055	0.92	0/1441
1	N	0.78	0/1033	0.92	0/1410
1	O	0.77	0/963	0.90	0/1313
1	P	0.79	0/957	0.94	0/1306
1	Q	0.80	0/1006	0.92	0/1372
1	R	0.83	0/978	0.91	0/1335
1	S	0.79	0/1064	0.90	0/1452
1	T	0.75	0/1070	0.94	0/1459
1	U	0.80	0/981	0.94	0/1335
1	V	0.79	0/951	0.97	0/1297
1	X	0.82	0/1008	0.96	1/1373 (0.1%)
1	Y	0.81	0/1006	0.92	0/1373
All	All	0.88	2/24828 (0.0%)	0.96	9/33860 (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	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	71	VAL	CA-CB	5.75	1.61	1.54
1	L	116	VAL	CA-CB	5.75	1.61	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	11	GLN	N-CA-C	7.28	120.48	109.41
1	G	25	ASN	N-CA-C	6.26	118.91	111.71
1	X	58	LEU	N-CA-C	-6.18	103.48	111.02
1	L	33	ASP	CA-C-N	5.93	125.80	119.28
1	L	33	ASP	C-N-CA	5.93	125.80	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	10	LEU	Peptide

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	1033	0	991	22	0
1	B	1008	0	973	11	0
1	C	1051	0	1023	21	0
1	D	1032	0	994	12	0
1	E	1053	0	1014	20	0
1	F	1040	0	1006	15	0
1	G	1022	0	975	26	0
1	H	1017	0	978	13	0
1	I	1042	0	1011	22	0
1	J	1055	0	1026	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1050	0	1010	15	0
1	L	1040	0	1003	9	0
1	M	1030	0	977	23	0
1	N	1009	0	969	19	0
1	O	941	0	901	24	0
1	P	937	0	895	31	0
1	Q	983	0	938	29	0
1	R	957	0	915	28	0
1	S	1039	0	997	16	0
1	T	1045	0	1008	23	0
1	U	959	0	930	32	0
1	V	929	0	897	29	0
1	X	986	0	949	21	0
1	Y	983	0	945	34	0
2	B	4	0	8	2	0
2	C	4	0	8	0	0
2	D	4	0	8	1	0
2	E	8	0	16	0	0
2	F	4	0	8	0	0
2	G	4	0	8	1	0
2	I	4	0	8	0	0
2	J	4	0	8	1	0
2	K	8	0	16	0	0
3	F	6	0	8	0	0
3	L	6	0	8	0	0
4	A	25	0	0	3	0
4	B	16	0	0	1	0
4	C	12	0	0	0	0
4	D	23	0	0	1	0
4	E	17	0	0	1	0
4	F	17	0	0	1	0
4	G	12	0	0	1	0
4	H	20	0	0	0	0
4	I	16	0	0	1	0
4	J	27	0	0	0	0
4	K	13	0	0	2	0
4	L	25	0	0	0	0
4	M	9	0	0	0	0
4	N	9	0	0	0	0
4	O	1	0	0	0	0
4	P	6	0	0	0	0
4	Q	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	6	0	0	0	0
4	S	5	0	0	0	0
4	T	4	0	0	0	0
4	U	3	0	0	1	0
4	V	7	0	0	0	0
4	X	6	0	0	0	0
4	Y	3	0	0	0	0
All	All	24586	0	23429	477	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 10.

The worst 5 of 477 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:C:4:LEU:HD23	1:C:10:LEU:HD12	1.44	0.98
1:P:79:VAL:HG21	1:P:93:VAL:HG13	1.49	0.94
1:V:64:THR:OG1	1:V:67:GLU:CB	2.22	0.87
1:I:59:LEU:HD11	1:I:122:LEU:HD21	1.58	0.83
1:G:59:LEU:HD21	1:G:122:LEU:HD21	1.60	0.83

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	129/140 (92%)	118 (92%)	10 (8%)	1 (1%)	16	34
1	B	122/140 (87%)	115 (94%)	7 (6%)	0	100	100
1	C	130/140 (93%)	127 (98%)	1 (1%)	2 (2%)	8	18
1	D	129/140 (92%)	124 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	131/140 (94%)	124 (95%)	7 (5%)	0	100	100
1	F	129/140 (92%)	123 (95%)	6 (5%)	0	100	100
1	G	126/140 (90%)	110 (87%)	14 (11%)	2 (2%)	7	16
1	H	124/140 (89%)	118 (95%)	6 (5%)	0	100	100
1	I	129/140 (92%)	122 (95%)	6 (5%)	1 (1%)	16	34
1	J	131/140 (94%)	127 (97%)	4 (3%)	0	100	100
1	K	130/140 (93%)	125 (96%)	4 (3%)	1 (1%)	16	34
1	L	130/140 (93%)	123 (95%)	7 (5%)	0	100	100
1	M	130/140 (93%)	117 (90%)	12 (9%)	1 (1%)	16	34
1	N	124/140 (89%)	110 (89%)	13 (10%)	1 (1%)	16	34
1	O	112/140 (80%)	100 (89%)	8 (7%)	4 (4%)	2	4
1	P	115/140 (82%)	100 (87%)	14 (12%)	1 (1%)	14	30
1	Q	121/140 (86%)	104 (86%)	15 (12%)	2 (2%)	7	15
1	R	119/140 (85%)	101 (85%)	13 (11%)	5 (4%)	2	3
1	S	130/140 (93%)	120 (92%)	10 (8%)	0	100	100
1	T	130/140 (93%)	121 (93%)	8 (6%)	1 (1%)	16	34
1	U	116/140 (83%)	104 (90%)	10 (9%)	2 (2%)	7	15
1	V	115/140 (82%)	95 (83%)	20 (17%)	0	100	100
1	X	118/140 (84%)	105 (89%)	13 (11%)	0	100	100
1	Y	120/140 (86%)	106 (88%)	13 (11%)	1 (1%)	16	34
All	All	2990/3360 (89%)	2739 (92%)	226 (8%)	25 (1%)	16	34

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	C	29	SER
1	G	32	GLU
1	I	6	GLY
1	Q	7	ASN

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	110/122 (90%)	99 (90%)	11 (10%)	7	16
1	B	109/122 (89%)	101 (93%)	8 (7%)	13	29
1	C	114/122 (93%)	105 (92%)	9 (8%)	11	26
1	D	110/122 (90%)	103 (94%)	7 (6%)	16	35
1	E	112/122 (92%)	105 (94%)	7 (6%)	16	36
1	F	112/122 (92%)	110 (98%)	2 (2%)	51	76
1	G	108/122 (88%)	93 (86%)	15 (14%)	3	7
1	H	109/122 (89%)	100 (92%)	9 (8%)	10	23
1	I	112/122 (92%)	105 (94%)	7 (6%)	16	36
1	J	113/122 (93%)	106 (94%)	7 (6%)	16	36
1	K	112/122 (92%)	101 (90%)	11 (10%)	7	17
1	L	112/122 (92%)	109 (97%)	3 (3%)	39	67
1	M	109/122 (89%)	101 (93%)	8 (7%)	13	29
1	N	108/122 (88%)	99 (92%)	9 (8%)	10	23
1	O	101/122 (83%)	92 (91%)	9 (9%)	9	20
1	P	99/122 (81%)	89 (90%)	10 (10%)	7	15
1	Q	104/122 (85%)	95 (91%)	9 (9%)	9	21
1	R	102/122 (84%)	90 (88%)	12 (12%)	5	10
1	S	111/122 (91%)	102 (92%)	9 (8%)	11	24
1	T	112/122 (92%)	100 (89%)	12 (11%)	6	14
1	U	103/122 (84%)	90 (87%)	13 (13%)	4	9
1	V	97/122 (80%)	89 (92%)	8 (8%)	10	24
1	X	106/122 (87%)	102 (96%)	4 (4%)	29	56
1	Y	106/122 (87%)	95 (90%)	11 (10%)	7	14
All	All	2591/2928 (88%)	2381 (92%)	210 (8%)	11	24

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	66	GLU
1	R	57	GLN

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Mol	Chain	Res	Type
1	Y	29	SER
1	O	109	THR
1	P	122	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	27	ASN
1	V	49	GLN
1	S	49	GLN
1	U	11	GLN
1	V	127	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
2	IPA	K	141	-	3,3,3	0.63	0	3,3,3	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IPA	C	141	-	3,3,3	0.63	0	3,3,3	0.30	0
2	IPA	K	142	-	3,3,3	0.40	0	3,3,3	0.50	0
3	GOL	F	141	-	5,5,5	0.98	0	5,5,5	1.49	1 (20%)
2	IPA	D	141	-	3,3,3	0.55	0	3,3,3	0.27	0
2	IPA	E	141	-	3,3,3	0.63	0	3,3,3	0.29	0
3	GOL	L	141	-	5,5,5	0.90	0	5,5,5	1.06	0
2	IPA	E	142	-	3,3,3	0.64	0	3,3,3	0.42	0
2	IPA	G	141	-	3,3,3	0.69	0	3,3,3	0.26	0
2	IPA	I	141	-	3,3,3	0.53	0	3,3,3	0.47	0
2	IPA	F	142	-	3,3,3	0.54	0	3,3,3	0.43	0
2	IPA	B	141	-	3,3,3	0.56	0	3,3,3	0.23	0
2	IPA	J	141	-	3,3,3	0.61	0	3,3,3	0.40	0

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	GOL	F	141	-	-	2/4/4/4	-
3	GOL	L	141	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	141	GOL	O1-C1-C2	2.07	119.68	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	141	GOL	O1-C1-C2-O2
3	F	141	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	141	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	141	IPA	1	0
2	B	141	IPA	2	0
2	J	141	IPA	1	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 ⓘ

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, 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	131/140 (93%)	-1.59	0 100 100	35, 59, 71, 74	0
1	B	126/140 (90%)	-1.69	0 100 100	29, 47, 62, 66	0
1	C	131/140 (93%)	-1.72	0 100 100	33, 48, 65, 72	1 (0%)
1	D	131/140 (93%)	-1.68	0 100 100	30, 48, 62, 67	0
1	E	132/140 (94%)	-1.68	0 100 100	24, 54, 68, 70	1 (0%)
1	F	131/140 (93%)	-1.68	0 100 100	36, 49, 61, 67	0
1	G	130/140 (92%)	-1.64	0 100 100	30, 59, 72, 75	0
1	H	128/140 (91%)	-1.67	0 100 100	28, 47, 63, 65	0
1	I	131/140 (93%)	-1.69	0 100 100	35, 48, 64, 73	0
1	J	132/140 (94%)	-1.66	0 100 100	24, 49, 63, 73	1 (0%)
1	K	131/140 (93%)	-1.65	0 100 100	23, 54, 67, 71	1 (0%)
1	L	131/140 (93%)	-1.67	0 100 100	29, 48, 62, 67	1 (0%)
1	M	132/140 (94%)	-1.66	0 100 100	49, 64, 86, 90	0
1	N	128/140 (91%)	-1.65	0 100 100	51, 64, 75, 82	0
1	O	118/140 (84%)	-1.60	0 100 100	31, 66, 79, 93	0
1	P	121/140 (86%)	-1.63	0 100 100	32, 68, 79, 91	0
1	Q	125/140 (89%)	-1.64	0 100 100	31, 66, 75, 88	0
1	R	123/140 (87%)	-1.65	0 100 100	31, 67, 79, 95	0
1	S	132/140 (94%)	-1.66	0 100 100	49, 63, 85, 87	0
1	T	132/140 (94%)	-1.62	0 100 100	31, 65, 78, 82	0
1	U	120/140 (85%)	-1.61	0 100 100	32, 68, 79, 86	0
1	V	119/140 (85%)	-1.60	0 100 100	32, 68, 76, 80	0
1	X	124/140 (88%)	-1.59	0 100 100	50, 66, 77, 90	0
1	Y	124/140 (88%)	-1.63	0 100 100	32, 68, 82, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3063/3360 (91%)	-1.65	0 100 100	23, 59, 77, 95	5 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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	GOL	F	141	6/6	0.98	0.06	47,50,51,51	0
2	IPA	C	141	4/4	0.99	0.03	35,35,38,39	0
2	IPA	D	141	4/4	0.99	0.03	39,40,42,43	0
2	IPA	E	141	4/4	0.99	0.03	35,40,40,41	0
2	IPA	E	142	4/4	0.99	0.05	34,35,37,38	0
2	IPA	F	142	4/4	0.99	0.03	28,30,31,32	0
2	IPA	G	141	4/4	0.99	0.04	43,43,45,46	0
2	IPA	I	141	4/4	0.99	0.04	33,35,36,36	0
2	IPA	J	141	4/4	0.99	0.03	37,38,39,40	0
2	IPA	K	141	4/4	0.99	0.04	30,34,34,35	0
2	IPA	K	142	4/4	0.99	0.04	33,35,35,36	0
2	IPA	B	141	4/4	0.99	0.04	47,47,48,48	0
3	GOL	L	141	6/6	0.99	0.05	49,53,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.