



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 PM GMT

PDB ID : 4FMG  
Title : Merkel Cell Polyomavirus VP1 Unassembled Pentamer  
Authors : Neu, U.; Hengel, H.; Stehle, T.  
Deposited on : 2012-06-17  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

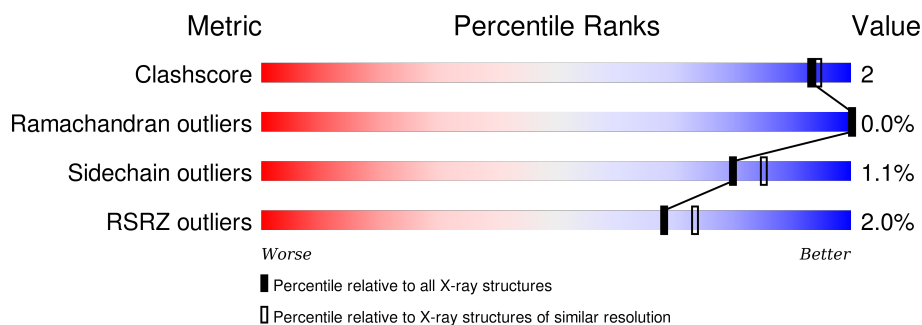
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	289	<div> <div>3%</div> <div>90%</div> <div>6%</div> </div>
1	B	289	<div> <div>3%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	C	289	<div> <div>%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	289	<div> <div>%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	E	289	<div> <div>%</div> <div>90%</div> <div>.</div> <div>6%</div> </div>
1	F	289	<div> <div>2%</div> <div>89%</div> <div>.</div> <div>6%</div> </div>
1	G	289	<div> <div>2%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	289	
1	I	289	
1	J	289	
1	K	289	
1	L	289	
1	M	289	
1	N	289	
1	O	289	
1	P	289	
1	Q	289	
1	R	289	
1	S	289	
1	T	289	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	501	-	-	X	X
2	GOL	A	503	-	-	-	X
2	GOL	B	402	-	-	-	X
2	GOL	C	402	-	-	-	X
2	GOL	D	501	-	-	-	X
2	GOL	F	402	-	-	-	X
2	GOL	H	402	-	-	-	X
2	GOL	I	402	-	-	-	X
2	GOL	J	402	-	-	-	X
2	GOL	L	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46380 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	6	0
			2154	1376	356	412	10			
1	B	273	Total	C	N	O	S	0	6	0
			2172	1386	360	416	10			
1	C	276	Total	C	N	O	S	0	5	0
			2186	1394	362	419	11			
1	D	271	Total	C	N	O	S	0	2	0
			2130	1359	353	407	11			
1	E	271	Total	C	N	O	S	0	3	0
			2135	1364	354	407	10			
1	F	272	Total	C	N	O	S	0	2	0
			2134	1363	353	408	10			
1	G	271	Total	C	N	O	S	0	5	0
			2146	1369	355	412	10			
1	H	277	Total	C	N	O	S	0	5	0
			2194	1399	363	421	11			
1	I	271	Total	C	N	O	S	0	4	0
			2140	1366	355	409	10			
1	J	271	Total	C	N	O	S	0	3	0
			2141	1368	354	409	10			
1	K	272	Total	C	N	O	S	0	4	0
			2152	1375	356	411	10			
1	L	270	Total	C	N	O	S	0	2	0
			2121	1354	351	406	10			
1	M	269	Total	C	N	O	S	0	2	0
			2116	1353	350	403	10			
1	N	270	Total	C	N	O	S	0	4	0
			2133	1363	353	407	10			
1	O	270	Total	C	N	O	S	0	1	0
			2114	1352	349	403	10			
1	P	273	Total	C	N	O	S	0	4	0
			2159	1377	357	415	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	271	Total	C	N	O	S	0	3	0
			2139	1367	354	408	10			
1	R	270	Total	C	N	O	S	0	1	0
			2114	1352	350	402	10			
1	S	271	Total	C	N	O	S	0	5	0
			2153	1374	359	410	10			
1	T	270	Total	C	N	O	S	0	6	0
			2161	1379	360	412	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
A	33	SER	-	EXPRESSION TAG	UNP C0JPK1
A	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
A	35	MET	-	EXPRESSION TAG	UNP C0JPK1
A	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
A	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
B	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
B	33	SER	-	EXPRESSION TAG	UNP C0JPK1
B	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
B	35	MET	-	EXPRESSION TAG	UNP C0JPK1
B	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
B	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
C	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
C	33	SER	-	EXPRESSION TAG	UNP C0JPK1
C	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
C	35	MET	-	EXPRESSION TAG	UNP C0JPK1
C	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
C	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
D	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
D	33	SER	-	EXPRESSION TAG	UNP C0JPK1
D	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
D	35	MET	-	EXPRESSION TAG	UNP C0JPK1
D	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
D	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
E	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
E	33	SER	-	EXPRESSION TAG	UNP C0JPK1
E	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
E	35	MET	-	EXPRESSION TAG	UNP C0JPK1
E	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
E	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
F	32	GLY	-	EXPRESSION TAG	UNP C0JPK1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	33	SER	-	EXPRESSION TAG	UNP C0JPK1
F	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
F	35	MET	-	EXPRESSION TAG	UNP C0JPK1
F	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
F	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
G	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
G	33	SER	-	EXPRESSION TAG	UNP C0JPK1
G	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
G	35	MET	-	EXPRESSION TAG	UNP C0JPK1
G	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
G	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
H	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
H	33	SER	-	EXPRESSION TAG	UNP C0JPK1
H	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
H	35	MET	-	EXPRESSION TAG	UNP C0JPK1
H	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
H	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
I	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
I	33	SER	-	EXPRESSION TAG	UNP C0JPK1
I	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
I	35	MET	-	EXPRESSION TAG	UNP C0JPK1
I	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
I	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
J	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
J	33	SER	-	EXPRESSION TAG	UNP C0JPK1
J	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
J	35	MET	-	EXPRESSION TAG	UNP C0JPK1
J	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
J	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
K	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
K	33	SER	-	EXPRESSION TAG	UNP C0JPK1
K	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
K	35	MET	-	EXPRESSION TAG	UNP C0JPK1
K	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
K	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
L	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
L	33	SER	-	EXPRESSION TAG	UNP C0JPK1
L	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
L	35	MET	-	EXPRESSION TAG	UNP C0JPK1
L	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
L	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
M	32	GLY	-	EXPRESSION TAG	UNP C0JPK1

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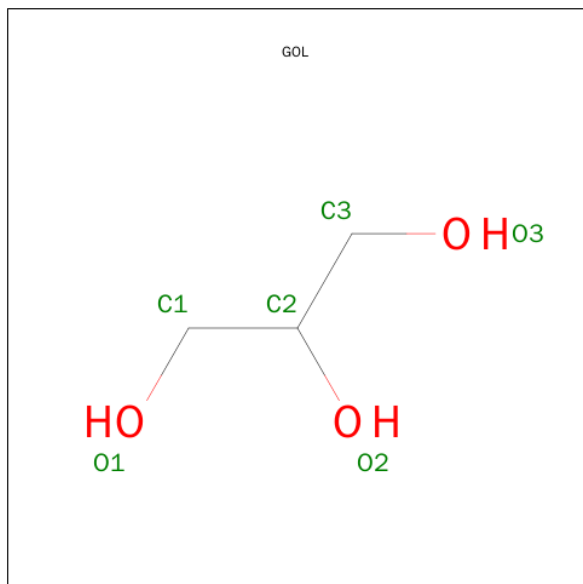
Chain	Residue	Modelled	Actual	Comment	Reference
M	33	SER	-	EXPRESSION TAG	UNP C0JPK1
M	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
M	35	MET	-	EXPRESSION TAG	UNP C0JPK1
M	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
M	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
N	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
N	33	SER	-	EXPRESSION TAG	UNP C0JPK1
N	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
N	35	MET	-	EXPRESSION TAG	UNP C0JPK1
N	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
N	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
O	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
O	33	SER	-	EXPRESSION TAG	UNP C0JPK1
O	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
O	35	MET	-	EXPRESSION TAG	UNP C0JPK1
O	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
O	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
P	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
P	33	SER	-	EXPRESSION TAG	UNP C0JPK1
P	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
P	35	MET	-	EXPRESSION TAG	UNP C0JPK1
P	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
P	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
Q	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
Q	33	SER	-	EXPRESSION TAG	UNP C0JPK1
Q	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
Q	35	MET	-	EXPRESSION TAG	UNP C0JPK1
Q	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
Q	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
R	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
R	33	SER	-	EXPRESSION TAG	UNP C0JPK1
R	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
R	35	MET	-	EXPRESSION TAG	UNP C0JPK1
R	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
R	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
S	32	GLY	-	EXPRESSION TAG	UNP C0JPK1
S	33	SER	-	EXPRESSION TAG	UNP C0JPK1
S	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
S	35	MET	-	EXPRESSION TAG	UNP C0JPK1
S	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
S	37	GLU	-	EXPRESSION TAG	UNP C0JPK1
T	32	GLY	-	EXPRESSION TAG	UNP C0JPK1

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Chain	Residue	Modelled	Actual	Comment	Reference
T	33	SER	-	EXPRESSION TAG	UNP C0JPK1
T	34	HIS	-	EXPRESSION TAG	UNP C0JPK1
T	35	MET	-	EXPRESSION TAG	UNP C0JPK1
T	36	LEU	-	EXPRESSION TAG	UNP C0JPK1
T	37	GLU	-	EXPRESSION TAG	UNP C0JPK1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	S	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	Q	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	K	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	T	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		
3	O	1	Total	Cl	0	0
			1	1		
3	R	1	Total	Cl	0	0
			1	1		
3	L	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	M	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total 153	O 153	0	0
4	B	163	Total 163	O 163	0	0
4	C	172	Total 172	O 172	0	0
4	D	170	Total 170	O 170	0	0
4	E	174	Total 174	O 174	0	0
4	F	145	Total 145	O 145	0	0
4	G	179	Total 179	O 179	0	0
4	H	163	Total 163	O 163	0	0
4	I	146	Total 146	O 146	0	0
4	J	153	Total 153	O 153	0	0
4	K	129	Total 129	O 129	0	0
4	L	165	Total 165	O 165	0	0
4	M	182	Total 182	O 182	0	0
4	N	161	Total 161	O 161	0	0
4	O	148	Total 148	O 148	0	0
4	P	175	Total 175	O 175	0	0

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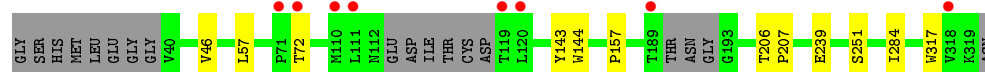
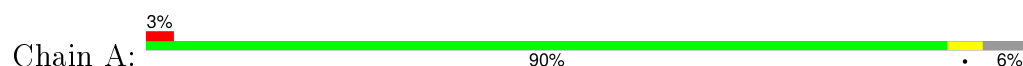
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	169	Total 169	O 169	0	0
4	R	195	Total 195	O 195	0	0
4	S	179	Total 179	O 179	0	0
4	T	153	Total 153	O 153	0	0

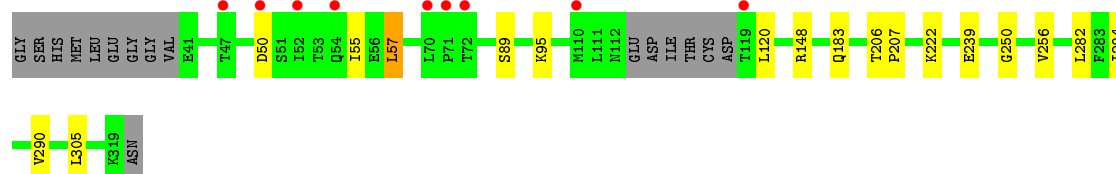
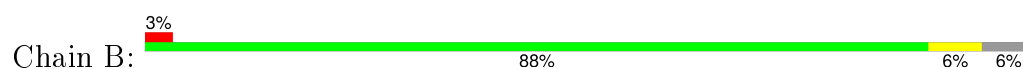
### 3 Residue-property plots [i](#)

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

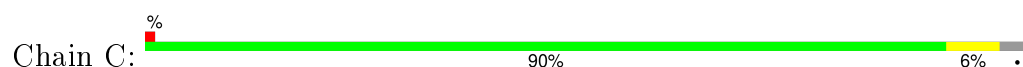
- Molecule 1: VP1



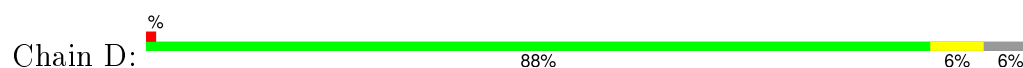
- Molecule 1: VP1



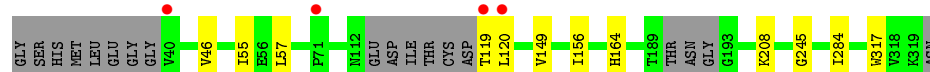
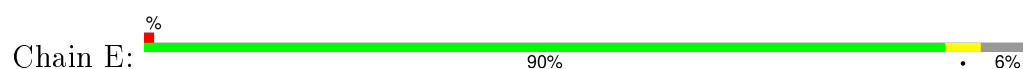
- Molecule 1: VP1



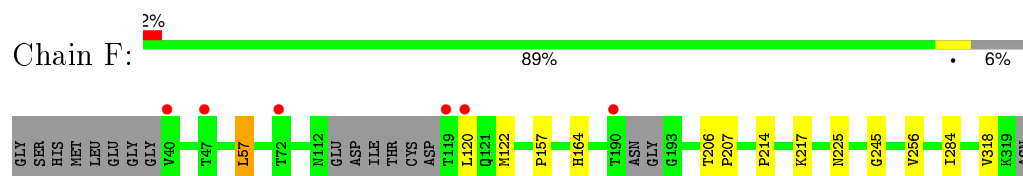
- Molecule 1: VP1



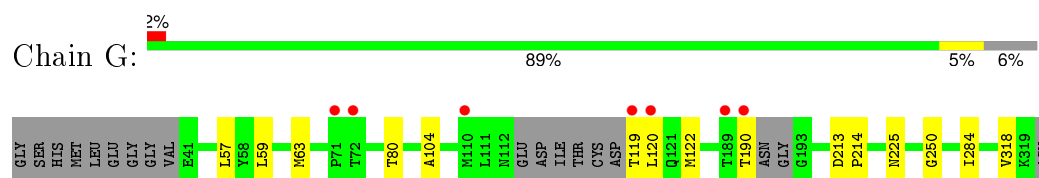
- Molecule 1: VP1



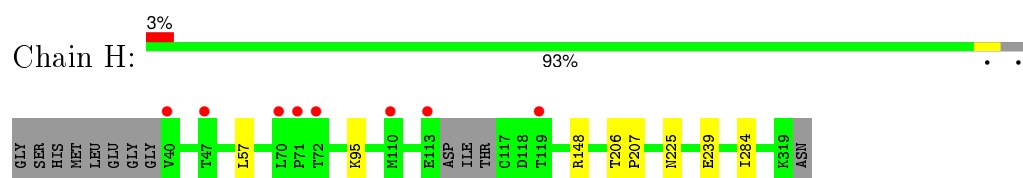
- Molecule 1: VP1



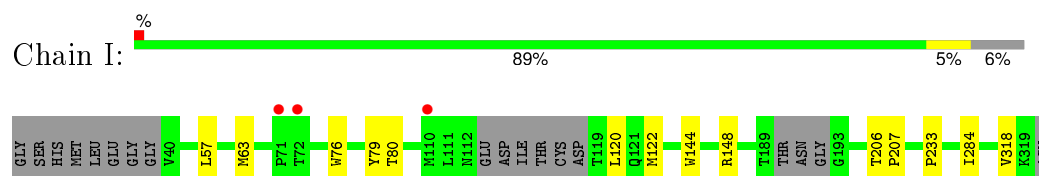
- Molecule 1: VP1



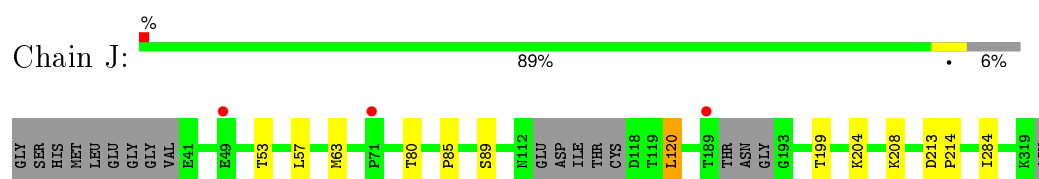
- Molecule 1: VP1



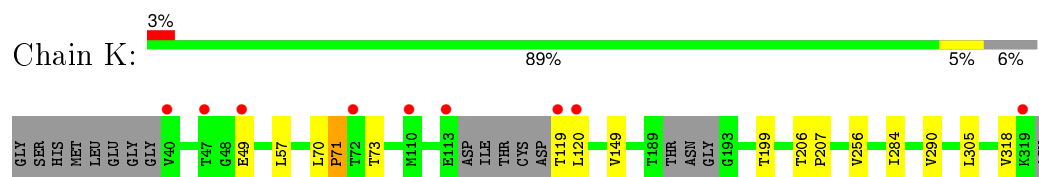
- Molecule 1: VP1



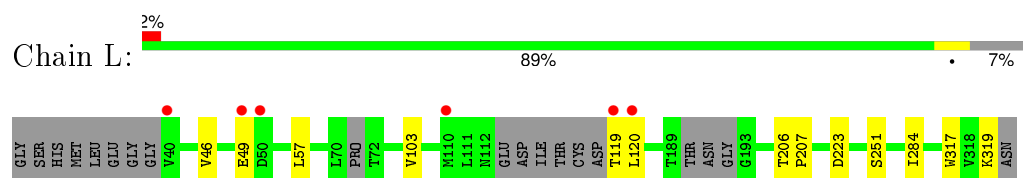
- Molecule 1: VP1



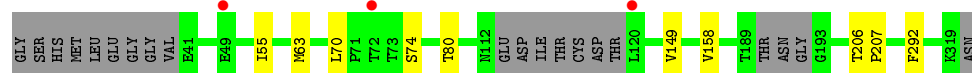
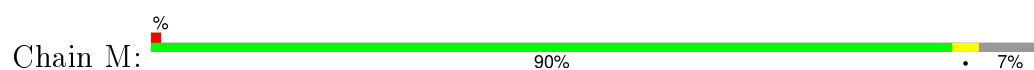
- Molecule 1: VP1



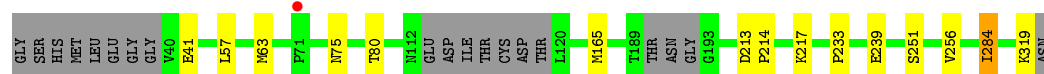
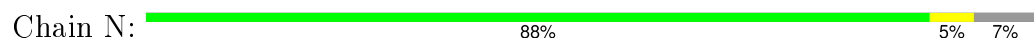
- Molecule 1: VP1



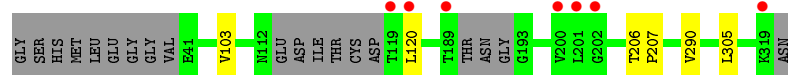
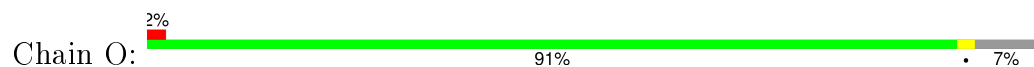
- Molecule 1: VP1



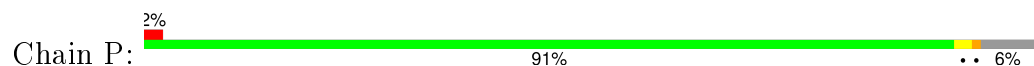
- Molecule 1: VP1



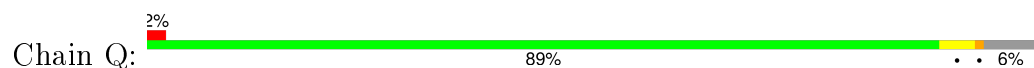
- Molecule 1: VP1



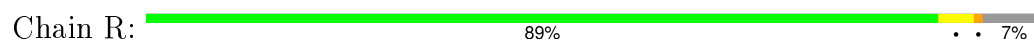
- Molecule 1: VP1



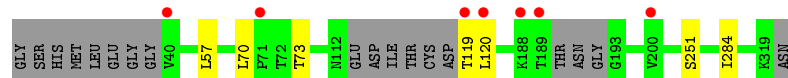
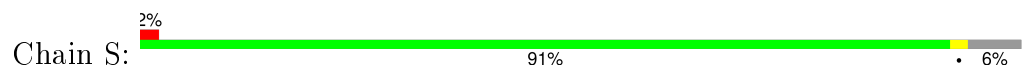
- Molecule 1: VP1



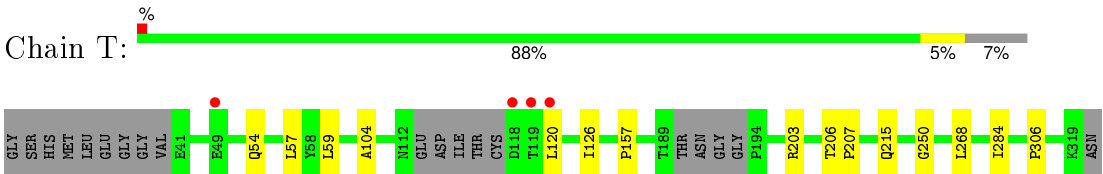
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.27Å 85.62Å 248.17Å 92.98° 100.50° 108.05°	Depositor
Resolution (Å)	50.00 – 2.10 43.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.10) 90.0 (43.88-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.182 , 0.227 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.7	EDS
Estimated twinning fraction	0.000 for k,h,-h-k-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 351166 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	46380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 21.48 % 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 6.9502e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL

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	0.41	0/2205	0.55	0/3004
1	B	0.42	0/2224	0.54	0/3032
1	C	0.43	0/2238	0.55	0/3052
1	D	0.44	0/2179	0.55	0/2965
1	E	0.44	0/2189	0.56	0/2981
1	F	0.43	0/2185	0.55	0/2978
1	G	0.41	0/2200	0.53	0/2997
1	H	0.42	0/2249	0.55	0/3066
1	I	0.42	0/2191	0.52	0/2985
1	J	0.42	0/2192	0.57	1/2986 (0.0%)
1	K	0.41	0/2206	0.55	0/3005
1	L	0.42	0/2170	0.52	0/2954
1	M	0.43	0/2167	0.54	0/2952
1	N	0.41	0/2184	0.55	0/2976
1	O	0.40	0/2165	0.53	0/2950
1	P	0.42	0/2210	0.56	0/3012
1	Q	0.42	0/2190	0.55	0/2984
1	R	0.43	0/2165	0.55	0/2949
1	S	0.43	0/2204	0.54	0/3003
1	T	0.40	0/2215	0.54	0/3016
All	All	0.42	0/43928	0.54	1/59847 (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	J	120	LEU	CA-CB-CG	5.69	128.38	115.30

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	2154	0	2136	9	0
1	B	2172	0	2158	17	0
1	C	2186	0	2169	14	0
1	D	2130	0	2107	12	0
1	E	2135	0	2123	10	0
1	F	2134	0	2111	9	0
1	G	2146	0	2129	9	0
1	H	2194	0	2176	5	0
1	I	2140	0	2117	8	0
1	J	2141	0	2125	7	0
1	K	2152	0	2135	9	0
1	L	2121	0	2106	8	0
1	M	2116	0	2104	8	0
1	N	2133	0	2116	9	0
1	O	2114	0	2097	2	0
1	P	2159	0	2140	7	0
1	Q	2139	0	2126	7	0
1	R	2114	0	2099	10	0
1	S	2153	0	2136	4	0
1	T	2161	0	2146	9	0
2	A	18	0	24	5	0
2	B	12	0	16	1	0
2	C	12	0	16	3	0
2	D	12	0	16	3	0
2	E	6	0	8	0	0
2	F	12	0	16	1	0
2	G	6	0	8	0	0
2	H	12	0	16	1	0
2	I	12	0	16	1	0
2	J	12	0	16	0	0
2	K	6	0	8	1	0
2	L	18	0	24	1	0
2	M	6	0	8	1	0
2	N	6	0	8	1	0
2	O	6	0	8	0	0
2	P	6	0	8	0	0
2	Q	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	6	0	8	0	0
2	S	12	0	16	0	0
2	T	6	0	8	1	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	1	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	1	0
4	A	153	0	0	0	0
4	B	163	0	0	1	0
4	C	172	0	0	2	0
4	D	170	0	0	1	0
4	E	174	0	0	3	0
4	F	145	0	0	0	0
4	G	179	0	0	0	0
4	H	163	0	0	0	0
4	I	146	0	0	0	0
4	J	153	0	0	2	0
4	K	129	0	0	0	0
4	L	165	0	0	0	0
4	M	182	0	0	1	0
4	N	161	0	0	0	0
4	O	148	0	0	0	0
4	P	175	0	0	3	0
4	Q	169	0	0	1	0
4	R	195	0	0	1	0
4	S	179	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	153	0	0	0	0
All	All	46380	0	42812	165	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 2.

All (165) 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:D:501:GOL:H32	4:E:645:HOH:O	1.35	1.24
1:B:55[B]:ILE:O	1:B:55[B]:ILE:HD12	1.54	1.07
1:Q:57[A]:LEU:HD21	1:Q:284:ILE:HD12	1.35	1.03
1:F:57:LEU:HD21	1:F:284:ILE:HD12	1.49	0.93
1:M:55[B]:ILE:HD12	1:M:55[B]:ILE:O	1.68	0.92
1:N:57:LEU:HD21	1:N:284:ILE:HD12	1.54	0.88
1:B:55[B]:ILE:O	1:B:55[B]:ILE:CD1	2.24	0.85
1:M:55[B]:ILE:C	1:M:55[B]:ILE:HD12	1.97	0.85
1:A:57[A]:LEU:HD21	1:A:284:ILE:HD12	1.56	0.85
1:B:57[A]:LEU:HD21	1:B:284:ILE:HD12	1.58	0.83
1:E:57:LEU:HD21	1:E:284:ILE:HD12	1.60	0.83
1:C:57[A]:LEU:HD21	1:C:284:ILE:HD13	1.62	0.81
1:J:57[A]:LEU:HD21	1:J:284:ILE:HD12	1.63	0.80
1:I:57:LEU:HD21	1:I:284:ILE:HD12	1.63	0.79
1:E:119:THR:HG21	1:K:119:THR:HG21	1.63	0.79
1:P:57:LEU:HD21	1:P:284:ILE:HD12	1.66	0.78
1:D:57:LEU:HD21	1:D:284:ILE:HD12	1.66	0.77
1:C:148:ARG:O	2:C:402:GOL:H12	1.84	0.77
2:L:501:GOL:H32	4:M:583:HOH:O	1.85	0.77
1:K:57[A]:LEU:HD21	1:K:284:ILE:HD13	1.66	0.75
1:R:57:LEU:HD21	1:R:284:ILE:HD12	1.66	0.75
1:L:57:LEU:HD21	1:L:284:ILE:HD13	1.73	0.69
1:S:57:LEU:HD21	1:S:284:ILE:HD13	1.74	0.68
1:B:55[B]:ILE:HD12	1:B:55[B]:ILE:C	2.15	0.66
1:G:119:THR:HG21	1:S:119:THR:HG21	1.78	0.65
1:B:55[B]:ILE:O	1:B:55[B]:ILE:CG1	2.46	0.64
1:I:57:LEU:HD21	1:I:284:ILE:CD1	2.27	0.64
1:H:57[A]:LEU:HD21	1:H:284:ILE:HD13	1.81	0.63
1:D:57:LEU:HD21	1:D:284:ILE:CD1	2.29	0.62
2:A:501:GOL:H11	4:B:556:HOH:O	1.98	0.62
1:E:57:LEU:HD21	1:E:284:ILE:CD1	2.29	0.61
1:E:57:LEU:CD2	1:E:284:ILE:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:57:LEU:HD21	1:T:284:ILE:HD13	1.82	0.61
1:K:290:VAL:HG11	1:K:305:LEU:HD12	1.84	0.60
1:F:206:THR:HB	1:F:207:PRO:HD2	1.84	0.60
1:C:148:ARG:O	2:C:402:GOL:C1	2.50	0.60
1:G:57:LEU:HD21	1:G:284:ILE:CD1	2.32	0.60
1:T:203[A]:ARG:NH2	1:T:215[A]:GLN:OE1	2.33	0.58
1:C:157:PRO:HG2	1:D:250:GLY:H	1.70	0.57
1:G:57:LEU:HD21	1:G:284:ILE:HD12	1.87	0.57
1:K:119:THR:HA	1:K:318:VAL:O	2.05	0.56
1:F:256:VAL:O	2:F:401:GOL:H11	2.05	0.56
1:F:157:PRO:HG2	1:G:250:GLY:H	1.71	0.56
1:F:57:LEU:HD21	1:F:284:ILE:CD1	2.30	0.55
1:P:250:GLY:H	1:T:157:PRO:HG2	1.72	0.54
1:H:206:THR:HB	1:H:207:PRO:HD2	1.88	0.54
2:T:401:GOL:O2	3:T:402:CL:CL	2.62	0.53
1:C:206:THR:HB	1:C:207:PRO:HD2	1.90	0.53
2:A:502:GOL:H2	3:A:504:CL:CL	2.45	0.53
1:K:57[A]:LEU:HD21	1:K:284:ILE:CD1	2.38	0.53
1:M:55[B]:ILE:C	1:M:55[B]:ILE:CD1	2.69	0.53
1:A:143:TYR:HE1	2:A:501:GOL:H2	1.74	0.53
1:P:190:THR:H	1:P:193:GLY:HA3	1.73	0.53
2:A:501:GOL:H31	1:B:183:GLN:OE1	2.09	0.52
1:T:206:THR:HB	1:T:207:PRO:HD2	1.90	0.52
1:T:57:LEU:HD21	1:T:284:ILE:CD1	2.39	0.52
1:O:290:VAL:HG11	1:O:305:LEU:HD12	1.90	0.52
1:L:206:THR:HB	1:L:207:PRO:HD2	1.91	0.52
1:N:256:VAL:O	2:N:401:GOL:H2	2.10	0.52
1:C:57[A]:LEU:CD2	1:C:284:ILE:HD13	2.37	0.51
2:A:501:GOL:C3	1:B:183:GLN:OE1	2.59	0.51
4:C:608:HOH:O	1:D:250:GLY:CA	2.58	0.51
1:J:204:LYS:HE2	4:J:587:HOH:O	2.10	0.51
1:T:59:LEU:HD21	1:T:104:ALA:HB2	1.92	0.51
1:H:57[A]:LEU:HD21	1:H:284:ILE:CD1	2.41	0.50
1:N:214:PRO:O	1:N:217:LYS:HE2	2.12	0.50
1:M:206:THR:HB	1:M:207:PRO:HD2	1.94	0.50
1:R:173:LEU:HD12	1:R:238:ASN:OD1	2.12	0.50
1:K:149:VAL:HG11	1:L:251:SER:HB3	1.93	0.49
1:F:122:MET:SD	1:F:318:VAL:HG21	2.52	0.49
1:H:57[A]:LEU:HD23	1:H:57[A]:LEU:N	2.28	0.49
1:B:55[B]:ILE:HG12	1:B:282:LEU:HD23	1.93	0.49
1:S:57:LEU:CD2	1:S:284:ILE:HD13	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:MET:O	1:J:80:THR:HG22	2.13	0.48
1:Q:111:LEU:HD21	1:Q:315:LYS:HE2	1.94	0.48
1:Q:149:VAL:HG11	1:R:251:SER:HB3	1.96	0.47
1:C:57[B]:LEU:HD13	1:C:57[B]:LEU:C	2.34	0.47
2:I:401:GOL:O2	3:I:403:CL:CL	2.66	0.47
1:I:206:THR:HB	1:I:207:PRO:HD2	1.96	0.47
4:C:608:HOH:O	1:D:250:GLY:HA3	2.14	0.47
1:I:148:ARG:NH1	1:J:85:PRO:O	2.48	0.47
1:A:57[A]:LEU:HD21	1:A:284:ILE:CD1	2.37	0.46
1:Q:57[A]:LEU:HD21	1:Q:284:ILE:CD1	2.26	0.46
1:B:256:VAL:O	2:B:401:GOL:H11	2.15	0.46
1:M:149:VAL:HG11	1:N:251:SER:HB3	1.98	0.46
1:M:70:LEU:O	1:M:74:SER:HB2	2.15	0.46
1:P:75[A]:ASN:ND2	4:P:601:HOH:O	2.45	0.46
1:K:256:VAL:O	2:K:401:GOL:H2	2.16	0.45
1:A:144:TRP:CE2	1:B:89[B]:SER:HB3	2.50	0.45
1:H:148:ARG:HB2	2:H:402:GOL:H12	1.98	0.45
1:P:278:LYS:HE3	4:P:655:HOH:O	2.15	0.45
1:R:270:GLU:CD	1:R:270:GLU:H	2.20	0.45
1:D:122:MET:SD	1:D:318:VAL:HG21	2.57	0.45
1:D:57:LEU:CD2	1:D:284:ILE:HD12	2.43	0.45
1:F:164:HIS:O	1:F:245:GLY:HA2	2.16	0.44
1:D:206:THR:HB	1:D:207:PRO:HD2	1.98	0.44
1:R:149:VAL:HG11	1:S:251:SER:HB2	2.00	0.44
1:J:208:LYS:HE3	4:J:575:HOH:O	2.16	0.44
1:F:57:LEU:CD2	1:F:284:ILE:HD12	2.35	0.44
1:I:122:MET:SD	1:I:318:VAL:HG21	2.57	0.44
1:N:41:GLU:HB3	1:N:319:LYS:HB2	2.00	0.44
1:E:164:HIS:O	1:E:245:GLY:HA2	2.18	0.44
1:G:213:ASP:HA	1:G:214:PRO:HD2	1.84	0.44
1:G:63:MET:O	1:G:80:THR:HG22	2.18	0.43
1:E:149:VAL:HG12	1:E:156:ILE:HG12	2.00	0.43
1:R:41:GLU:HG3	4:R:688:HOH:O	2.18	0.43
2:D:501:GOL:C3	4:E:645:HOH:O	2.21	0.43
1:M:63:MET:O	1:M:80:THR:HG22	2.19	0.43
1:L:119:THR:HA	1:L:319:LYS:HA	2.00	0.43
1:B:55[B]:ILE:CD1	1:B:55[B]:ILE:C	2.83	0.43
4:Q:647:HOH:O	1:R:250:GLY:HA2	2.18	0.43
1:A:251[A]:SER:HB3	1:E:149:VAL:HG11	2.00	0.43
1:N:63:MET:O	1:N:80:THR:HG22	2.18	0.43
1:B:148:ARG:HH12	1:C:84:GLN:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:206:THR:HB	1:K:207:PRO:HD2	2.00	0.43
1:E:208:LYS:HE3	4:E:653:HOH:O	2.19	0.43
1:F:214:PRO:O	1:F:217:LYS:HE2	2.19	0.43
1:B:290:VAL:HG11	1:B:305:LEU:HD12	2.00	0.43
1:I:144:TRP:CE2	1:J:89:SER:HB3	2.54	0.43
1:L:57:LEU:HD21	1:L:284:ILE:CD1	2.45	0.42
1:B:206:THR:HB	1:B:207:PRO:HD2	2.00	0.42
1:E:46:VAL:HG22	1:E:317:TRP:CD1	2.54	0.42
1:G:122:MET:SD	1:G:318:VAL:HG21	2.59	0.42
1:Q:206:THR:HB	1:Q:207:PRO:HD2	2.01	0.42
1:N:75:ASN:ND2	1:N:75:ASN:H	2.17	0.42
1:A:46:VAL:HG22	1:A:317:TRP:CD1	2.54	0.42
2:D:502:GOL:H2	3:D:503:CL:CL	2.57	0.42
1:T:126:ILE:HG22	1:T:268:LEU:HD21	2.01	0.42
1:R:206:THR:HB	1:R:207:PRO:CD	2.49	0.42
1:R:122:MET:HE3	1:R:278:LYS:HG3	2.01	0.42
1:J:213:ASP:HA	1:J:214:PRO:HD2	1.91	0.42
1:A:206:THR:HB	1:A:207:PRO:HD2	2.01	0.42
1:D:165:MET:HA	1:D:244:TYR:O	2.19	0.42
1:P:75[B]:ASN:HD22	1:P:75[B]:ASN:N	2.18	0.42
2:M:401:GOL:O2	3:M:402:CL:CL	2.71	0.41
1:C:59:LEU:HD21	1:C:104:ALA:HB2	2.01	0.41
4:S:580:HOH:O	1:T:250:GLY:HA2	2.19	0.41
1:N:213:ASP:HA	1:N:214:PRO:HD3	1.93	0.41
1:I:63:MET:O	1:I:80:THR:HG22	2.20	0.41
1:A:157:PRO:HG2	1:B:250:GLY:H	1.84	0.41
1:L:103:VAL:HG12	1:L:223:ASP:HA	2.02	0.41
1:O:206:THR:HB	1:O:207:PRO:HD2	2.02	0.41
1:C:171:GLU:HB2	1:C:172:PRO:HD2	2.03	0.41
1:C:49:GLU:OE2	1:L:49:GLU:HB2	2.20	0.41
1:B:55[B]:ILE:O	1:B:55[B]:ILE:HG13	2.18	0.41
1:C:149[A]:VAL:HG11	1:D:251:SER:HB3	2.01	0.41
4:P:513:HOH:O	1:T:306:PRO:HD3	2.21	0.41
1:G:57:LEU:HD21	1:G:284:ILE:HD13	2.00	0.41
1:C:63:MET:O	1:C:80:THR:HG22	2.20	0.41
1:Q:70:LEU:HD12	1:Q:71:PRO:HD2	2.03	0.41
1:D:164:HIS:O	1:D:245:GLY:HA2	2.21	0.41
1:B:55[B]:ILE:HG12	1:B:282:LEU:CD2	2.51	0.41
1:A:57[A]:LEU:N	1:A:57[A]:LEU:HD23	2.35	0.41
1:M:158:VAL:HA	1:M:292:PHE:O	2.20	0.41
1:L:46:VAL:HG22	1:L:317:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:LEU:HD21	1:G:104:ALA:HB2	2.03	0.41
1:R:122:MET:CE	1:R:278:LYS:HG3	2.51	0.40
1:Q:189:THR:O	1:Q:190:THR:HG23	2.20	0.40
1:I:76:TRP:O	1:I:79:TYR:HB2	2.22	0.40
1:E:55:ILE:HD13	1:E:55:ILE:HA	1.85	0.40
1:N:165:MET:CE	1:N:233:PRO:HG3	2.51	0.40
1:P:214:PRO:O	1:P:217:LYS:HE2	2.22	0.40
1:D:209:ASN:HA	4:D:648:HOH:O	2.20	0.40
1:C:151:ASP:OD1	2:C:402:GOL:H31	2.22	0.40
1:K:70:LEU:HB3	1:K:71:PRO:HD2	2.04	0.40

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	271/289 (94%)	257 (95%)	14 (5%)	0	100	100
1	B	275/289 (95%)	264 (96%)	11 (4%)	0	100	100
1	C	277/289 (96%)	263 (95%)	14 (5%)	0	100	100
1	D	265/289 (92%)	257 (97%)	8 (3%)	0	100	100
1	E	268/289 (93%)	258 (96%)	10 (4%)	0	100	100
1	F	268/289 (93%)	255 (95%)	13 (5%)	0	100	100
1	G	270/289 (93%)	260 (96%)	10 (4%)	0	100	100
1	H	278/289 (96%)	268 (96%)	10 (4%)	0	100	100
1	I	269/289 (93%)	259 (96%)	10 (4%)	0	100	100
1	J	268/289 (93%)	259 (97%)	9 (3%)	0	100	100
1	K	270/289 (93%)	254 (94%)	14 (5%)	2 (1%)	26	21
1	L	264/289 (91%)	251 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	265/289 (92%)	254 (96%)	11 (4%)	0	100	100
1	N	268/289 (93%)	258 (96%)	10 (4%)	0	100	100
1	O	265/289 (92%)	253 (96%)	12 (4%)	0	100	100
1	P	271/289 (94%)	261 (96%)	10 (4%)	0	100	100
1	Q	268/289 (93%)	255 (95%)	13 (5%)	0	100	100
1	R	265/289 (92%)	254 (96%)	11 (4%)	0	100	100
1	S	270/289 (93%)	258 (96%)	12 (4%)	0	100	100
1	T	270/289 (93%)	260 (96%)	10 (4%)	0	100	100
All	All	5385/5780 (93%)	5158 (96%)	225 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	71	PRO
1	K	49	GLU

### 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	244/253 (96%)	242 (99%)	2 (1%)	86	91
1	B	246/253 (97%)	239 (97%)	7 (3%)	51	55
1	C	248/253 (98%)	247 (100%)	1 (0%)	93	96
1	D	240/253 (95%)	236 (98%)	4 (2%)	68	74
1	E	241/253 (95%)	240 (100%)	1 (0%)	93	96
1	F	240/253 (95%)	237 (99%)	3 (1%)	76	82
1	G	244/253 (96%)	241 (99%)	3 (1%)	78	84
1	H	249/253 (98%)	246 (99%)	3 (1%)	78	84
1	I	241/253 (95%)	239 (99%)	2 (1%)	86	91
1	J	242/253 (96%)	239 (99%)	3 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	243/253 (96%)	240 (99%)	3 (1%)	78	84
1	L	240/253 (95%)	239 (100%)	1 (0%)	93	96
1	M	239/253 (94%)	239 (100%)	0	100	100
1	N	241/253 (95%)	239 (99%)	2 (1%)	86	91
1	O	238/253 (94%)	236 (99%)	2 (1%)	86	91
1	P	245/253 (97%)	240 (98%)	5 (2%)	63	68
1	Q	242/253 (96%)	237 (98%)	5 (2%)	61	66
1	R	238/253 (94%)	235 (99%)	3 (1%)	76	82
1	S	243/253 (96%)	240 (99%)	3 (1%)	78	84
1	T	245/253 (97%)	242 (99%)	3 (1%)	78	84
All	All	4849/5060 (96%)	4793 (99%)	56 (1%)	80	84

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	239	GLU
1	B	50	ASP
1	B	57[A]	LEU
1	B	57[B]	LEU
1	B	95	LYS
1	B	120	LEU
1	B	222	LYS
1	B	239	GLU
1	C	40	VAL
1	D	50	ASP
1	D	120	LEU
1	D	188	LYS
1	D	239	GLU
1	E	120	LEU
1	F	57	LEU
1	F	120	LEU
1	F	225	ASN
1	G	120	LEU
1	G	190	THR
1	G	225	ASN
1	H	95	LYS
1	H	225	ASN

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Mol	Chain	Res	Type
1	H	239	GLU
1	I	120	LEU
1	I	233	PRO
1	J	53	THR
1	J	120	LEU
1	J	199	THR
1	K	73	THR
1	K	120	LEU
1	K	199	THR
1	L	120	LEU
1	N	239	GLU
1	N	284	ILE
1	O	103	VAL
1	O	120	LEU
1	P	57	LEU
1	P	75[A]	ASN
1	P	75[B]	ASN
1	P	120	LEU
1	P	284	ILE
1	Q	50	ASP
1	Q	70	LEU
1	Q	120	LEU
1	Q	190	THR
1	Q	208	LYS
1	R	57	LEU
1	R	239	GLU
1	R	284	ILE
1	S	70	LEU
1	S	73	THR
1	S	120	LEU
1	T	54[A]	GLN
1	T	54[B]	GLN
1	T	120	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	F	252	GLN
1	G	225	ASN
1	I	75	ASN
1	I	183	GLN

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Mol	Chain	Res	Type
1	J	183	GLN
1	J	225	ASN
1	K	225	ASN
1	Q	215	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 20 are monoatomic - leaving 32 for Mogul analysis.

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	GOL	A	501	-	5,5,5	0.40	0	5,5,5	0.47	0
2	GOL	A	502	-	5,5,5	0.32	0	5,5,5	0.58	0
2	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.61	0
2	GOL	B	401	-	5,5,5	0.41	0	5,5,5	0.29	0
2	GOL	B	402	-	5,5,5	0.34	0	5,5,5	0.27	0
2	GOL	C	401	-	5,5,5	0.41	0	5,5,5	0.23	0
2	GOL	C	402	-	5,5,5	0.31	0	5,5,5	0.46	0
2	GOL	D	501	-	5,5,5	0.44	0	5,5,5	0.40	0
2	GOL	D	502	-	5,5,5	0.40	0	5,5,5	0.32	0
2	GOL	E	401	-	5,5,5	0.48	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	F	401	-	5,5,5	0.38	0	5,5,5	0.71	0
2	GOL	F	402	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	G	401	-	5,5,5	0.43	0	5,5,5	0.71	0
2	GOL	H	401	-	5,5,5	0.34	0	5,5,5	0.35	0
2	GOL	H	402	-	5,5,5	0.41	0	5,5,5	0.40	0
2	GOL	I	401	-	5,5,5	0.44	0	5,5,5	0.29	0
2	GOL	I	402	-	5,5,5	0.34	0	5,5,5	0.32	0
2	GOL	J	401	-	5,5,5	0.40	0	5,5,5	0.28	0
2	GOL	J	402	-	5,5,5	0.32	0	5,5,5	0.44	0
2	GOL	K	401	-	5,5,5	0.41	0	5,5,5	0.31	0
2	GOL	L	501	-	5,5,5	0.37	0	5,5,5	0.44	0
2	GOL	L	502	-	5,5,5	0.44	0	5,5,5	0.35	0
2	GOL	L	503	-	5,5,5	0.29	0	5,5,5	0.48	0
2	GOL	M	401	-	5,5,5	0.43	0	5,5,5	0.34	0
2	GOL	N	401	-	5,5,5	0.38	0	5,5,5	0.31	0
2	GOL	O	401	-	5,5,5	0.37	0	5,5,5	0.41	0
2	GOL	P	401	-	5,5,5	0.43	0	5,5,5	0.27	0
2	GOL	Q	401	-	5,5,5	0.29	0	5,5,5	0.37	0
2	GOL	R	401	-	5,5,5	0.46	0	5,5,5	0.32	0
2	GOL	S	401	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	S	402	-	5,5,5	0.25	0	5,5,5	0.43	0
2	GOL	T	401	-	5,5,5	0.36	0	5,5,5	0.44	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
2	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	GOL	D	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	502	-	-	0/4/4/4	0/0/0/0
2	GOL	E	401	-	-	0/4/4/4	0/0/0/0
2	GOL	F	401	-	-	0/4/4/4	0/0/0/0
2	GOL	F	402	-	-	0/4/4/4	0/0/0/0
2	GOL	G	401	-	-	0/4/4/4	0/0/0/0
2	GOL	H	401	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	H	402	-	-	0/4/4/4	0/0/0/0
2	GOL	I	401	-	-	0/4/4/4	0/0/0/0
2	GOL	I	402	-	-	0/4/4/4	0/0/0/0
2	GOL	J	401	-	-	0/4/4/4	0/0/0/0
2	GOL	J	402	-	-	0/4/4/4	0/0/0/0
2	GOL	K	401	-	-	0/4/4/4	0/0/0/0
2	GOL	L	501	-	-	0/4/4/4	0/0/0/0
2	GOL	L	502	-	-	0/4/4/4	0/0/0/0
2	GOL	L	503	-	-	0/4/4/4	0/0/0/0
2	GOL	M	401	-	-	0/4/4/4	0/0/0/0
2	GOL	N	401	-	-	0/4/4/4	0/0/0/0
2	GOL	O	401	-	-	0/4/4/4	0/0/0/0
2	GOL	P	401	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	401	-	-	0/4/4/4	0/0/0/0
2	GOL	R	401	-	-	0/4/4/4	0/0/0/0
2	GOL	S	401	-	-	0/4/4/4	0/0/0/0
2	GOL	S	402	-	-	0/4/4/4	0/0/0/0
2	GOL	T	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	4	0
2	A	502	GOL	1	0
2	B	401	GOL	1	0
2	C	402	GOL	3	0
2	D	501	GOL	2	0
2	D	502	GOL	1	0
2	F	401	GOL	1	0
2	H	402	GOL	1	0
2	I	401	GOL	1	0
2	K	401	GOL	1	0
2	L	501	GOL	1	0
2	M	401	GOL	1	0
2	N	401	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	401	GOL	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, 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	271/289 (93%)	0.01	8 (2%) 54 62	13, 23, 50, 70	0
1	B	273/289 (94%)	-0.10	9 (3%) 50 59	13, 23, 49, 74	0
1	C	276/289 (95%)	-0.17	4 (1%) 78 82	12, 21, 47, 76	0
1	D	271/289 (93%)	-0.25	4 (1%) 76 81	11, 19, 45, 81	0
1	E	271/289 (93%)	-0.23	4 (1%) 76 81	10, 21, 46, 69	0
1	F	272/289 (94%)	-0.22	6 (2%) 65 71	13, 23, 47, 81	0
1	G	271/289 (93%)	0.02	7 (2%) 59 66	12, 22, 46, 65	0
1	H	277/289 (95%)	-0.05	8 (2%) 55 63	13, 23, 49, 71	0
1	I	271/289 (93%)	-0.10	3 (1%) 82 86	13, 24, 46, 76	0
1	J	271/289 (93%)	-0.25	3 (1%) 82 86	14, 22, 49, 78	0
1	K	272/289 (94%)	-0.00	9 (3%) 50 59	15, 25, 54, 78	0
1	L	270/289 (93%)	-0.06	6 (2%) 65 71	13, 22, 41, 70	0
1	M	269/289 (93%)	-0.24	3 (1%) 82 86	13, 20, 41, 71	0
1	N	270/289 (93%)	-0.01	1 (0%) 93 94	14, 24, 51, 70	0
1	O	270/289 (93%)	-0.03	7 (2%) 59 66	15, 26, 50, 77	0
1	P	273/289 (94%)	0.07	7 (2%) 59 66	12, 22, 47, 65	0
1	Q	271/289 (93%)	-0.17	6 (2%) 65 71	12, 21, 48, 76	0
1	R	270/289 (93%)	-0.07	1 (0%) 93 94	13, 21, 40, 64	0
1	S	271/289 (93%)	-0.18	7 (2%) 59 66	12, 20, 44, 75	0
1	T	270/289 (93%)	-0.14	4 (1%) 76 81	14, 21, 45, 78	0
All	All	5430/5780 (93%)	-0.11	107 (1%) 68 73	10, 22, 48, 81	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	5.8
1	A	119	THR	5.4
1	K	72	THR	5.2
1	S	40	VAL	5.1
1	T	119	THR	4.9
1	C	49	GLU	4.6
1	S	119	THR	4.5
1	H	71	PRO	4.5
1	Q	71	PRO	4.3
1	P	40	VAL	4.2
1	T	49	GLU	4.2
1	G	110	MET	4.2
1	N	71	PRO	4.2
1	B	119	THR	4.2
1	K	119	THR	4.2
1	E	40	VAL	4.1
1	E	119	THR	4.1
1	Q	119	THR	4.1
1	T	118	ASP	4.1
1	G	119	THR	4.0
1	L	119	THR	4.0
1	O	119	THR	3.9
1	G	120	LEU	3.8
1	L	110	MET	3.8
1	G	189	THR	3.7
1	O	202	GLY	3.6
1	K	49	GLU	3.5
1	A	71	PRO	3.5
1	I	72	THR	3.5
1	E	71	PRO	3.5
1	M	72	THR	3.4
1	G	72	THR	3.4
1	F	119	THR	3.3
1	K	40	VAL	3.3
1	G	190	THR	3.3
1	H	119	THR	3.3
1	B	71	PRO	3.3
1	A	72	THR	3.2
1	L	40	VAL	3.2
1	P	110	MET	3.2
1	L	49	GLU	3.1
1	O	189	THR	3.1
1	O	200	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	49	GLU	3.1
1	B	52	ILE	3.1
1	P	71	PRO	3.1
1	A	189	THR	3.0
1	B	72	THR	3.0
1	P	119	THR	3.0
1	Q	189	THR	3.0
1	K	113	GLU	3.0
1	H	40	VAL	3.0
1	I	110	MET	3.0
1	S	200[A]	VAL	2.9
1	K	47	THR	2.8
1	Q	49	GLU	2.8
1	F	40	VAL	2.8
1	F	190	THR	2.8
1	O	319	LYS	2.7
1	C	40	VAL	2.7
1	K	110	MET	2.7
1	K	120	LEU	2.7
1	O	120	LEU	2.7
1	H	113	GLU	2.7
1	F	72	THR	2.7
1	C	72	THR	2.6
1	B	50	ASP	2.6
1	L	50	ASP	2.6
1	D	118	ASP	2.6
1	A	111	LEU	2.6
1	A	110	MET	2.5
1	C	71	PRO	2.5
1	T	120	LEU	2.5
1	O	201	LEU	2.5
1	S	120	LEU	2.5
1	H	110	MET	2.5
1	S	188	LYS	2.5
1	D	189	THR	2.4
1	J	189	THR	2.4
1	M	120	LEU	2.4
1	Q	110	MET	2.4
1	E	120	LEU	2.4
1	D	40	VAL	2.4
1	B	110	MET	2.4
1	H	47	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	120	LEU	2.4
1	I	71	PRO	2.3
1	H	72	THR	2.3
1	K	319	LYS	2.3
1	M	49	GLU	2.3
1	F	120	LEU	2.3
1	B	47	THR	2.2
1	J	71	PRO	2.2
1	Q	190	THR	2.2
1	B	70	LEU	2.2
1	H	70	LEU	2.1
1	P	50	ASP	2.1
1	F	47	THR	2.1
1	S	189	THR	2.1
1	S	71	PRO	2.1
1	R	40	VAL	2.1
1	P	190	THR	2.0
1	B	54[A]	GLN	2.0
1	G	71	PRO	2.0
1	J	49	GLU	2.0
1	A	318	VAL	2.0
1	P	49	GLU	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	H	402	6/6	0.91	0.30	19.57	39,41,43,50	0
2	GOL	L	501	6/6	0.95	0.22	14.21	19,26,32,39	0
2	GOL	B	402	6/6	0.89	0.20	11.70	29,46,47,52	0
2	GOL	D	501	6/6	0.94	0.21	8.74	21,25,29,33	0
2	GOL	A	503	6/6	0.90	0.21	8.00	37,47,48,50	0
2	GOL	J	402	6/6	0.88	0.17	6.94	44,46,47,49	0
2	GOL	I	402	6/6	0.83	0.16	5.10	49,51,55,56	0
2	GOL	A	501	6/6	0.92	0.26	4.96	28,30,35,38	0
2	GOL	C	402	6/6	0.86	0.18	4.87	42,44,46,49	0
2	GOL	F	402	6/6	0.93	0.14	3.88	30,33,36,41	0
2	GOL	S	401	6/6	0.96	0.18	1.69	21,31,31,35	0
2	GOL	B	401	6/6	0.95	0.12	1.16	27,35,37,37	0
2	GOL	L	503	6/6	0.88	0.12	0.16	37,38,42,42	0
2	GOL	F	401	6/6	0.96	0.11	0.13	22,29,34,38	0
2	GOL	S	402	6/6	0.95	0.10	0.10	24,27,29,30	0
2	GOL	K	401	6/6	0.96	0.10	-0.17	19,30,31,34	0
2	GOL	R	401	6/6	0.95	0.14	-0.44	21,34,35,37	0
2	GOL	E	401	6/6	0.98	0.10	-0.55	9,23,30,31	0
2	GOL	D	502	6/6	0.94	0.10	-0.87	21,27,30,33	0
2	GOL	J	401	6/6	0.96	0.08	-0.92	25,34,35,35	0
2	GOL	T	401	6/6	0.96	0.09	-0.93	17,26,28,36	0
2	GOL	N	401	6/6	0.96	0.10	-1.07	18,29,32,34	0
2	GOL	Q	401	6/6	0.96	0.10	-1.07	11,27,29,31	0
2	GOL	I	401	6/6	0.96	0.11	-1.22	16,27,28,33	0
2	GOL	C	401	6/6	0.96	0.09	-1.25	20,26,30,31	0
2	GOL	A	502	6/6	0.94	0.11	-1.53	21,31,31,36	0
2	GOL	M	401	6/6	0.97	0.08	-1.60	12,26,27,31	0
3	CL	B	403	1/1	0.99	0.04	-1.91	25,25,25,25	0
3	CL	J	403	1/1	0.99	0.05	-1.97	23,23,23,23	0
2	GOL	P	401	6/6	0.96	0.10	-2.21	22,31,32,34	0
2	GOL	L	502	6/6	0.95	0.10	-2.39	22,29,31,31	0
3	CL	N	402	1/1	1.00	0.03	-2.53	19,19,19,19	0
3	CL	F	403	1/1	1.00	0.04	-2.87	24,24,24,24	0
3	CL	Q	402	1/1	1.00	0.02	-3.02	22,22,22,22	0
2	GOL	G	401	6/6	0.97	0.09	-3.26	13,22,29,31	0
2	GOL	O	401	6/6	0.98	0.07	-3.41	13,29,33,33	0
3	CL	E	402	1/1	0.99	0.03	-3.45	19,19,19,19	0
3	CL	H	403	1/1	0.99	0.03	-3.60	21,21,21,21	0
3	CL	A	504	1/1	1.00	0.03	-3.66	22,22,22,22	0
3	CL	M	402	1/1	0.99	0.04	-3.88	25,25,25,25	0
2	GOL	H	401	6/6	0.98	0.06	-3.96	13,25,26,28	0
3	CL	K	402	1/1	0.99	0.02	-3.99	29,29,29,29	0
3	CL	C	403	1/1	0.99	0.05	-4.51	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	L	504	1/1	1.00	0.04	-4.71	21,21,21,21	0
3	CL	D	503	1/1	0.99	0.03	-4.75	20,20,20,20	0
3	CL	R	402	1/1	1.00	0.04	-4.92	20,20,20,20	0
3	CL	T	402	1/1	1.00	0.04	-5.01	18,18,18,18	0
3	CL	O	402	1/1	0.97	0.06	-5.38	24,24,24,24	0
3	CL	S	403	1/1	0.99	0.04	-5.86	20,20,20,20	0
3	CL	G	402	1/1	0.99	0.04	-6.02	23,23,23,23	0
3	CL	I	403	1/1	0.99	0.04	-6.11	24,24,24,24	0
3	CL	P	402	1/1	0.99	0.03	-6.86	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.