



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 02:34 AM GMT

PDB ID : 2DF7  
Title : Crystal structure of infectious bursal disease virus VP2 subviral particle  
Authors : Ko, T.P.; Lee, C.C.; Wang, M.Y.; Wang, A.H.  
Deposited on : 2006-02-27  
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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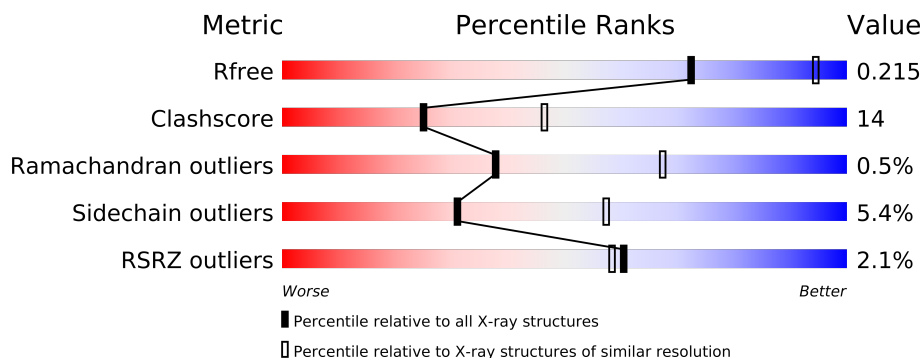
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	458	
1	B	458	
1	C	458	
1	D	458	
1	E	458	
1	F	458	
1	G	458	
1	H	458	
1	I	458	
1	J	458	
1	K	458	
1	L	458	
1	M	458	
1	N	458	

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Mol	Chain	Length	Quality of chain
1	O	458	
1	P	458	
1	Q	458	
1	R	458	
1	S	458	
1	T	458	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 66956 atoms, of which 0 are hydrogen and 0 are deuterium.

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 structural polyprotein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3162	2006	520	626	10			
1	B	418	Total	C	N	O	S	0	0	0
			3149	1997	518	624	10			
1	C	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	D	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	E	415	Total	C	N	O	S	0	0	0
			3130	1985	515	620	10			
1	F	413	Total	C	N	O	S	0	0	0
			3113	1974	513	616	10			
1	G	412	Total	C	N	O	S	0	0	0
			3110	1971	512	617	10			
1	H	413	Total	C	N	O	S	0	0	0
			3117	1976	513	618	10			
1	I	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	J	411	Total	C	N	O	S	0	0	0
			3102	1965	511	616	10			
1	K	417	Total	C	N	O	S	0	0	0
			3137	1988	517	622	10			
1	L	418	Total	C	N	O	S	0	0	0
			3150	1998	518	624	10			
1	M	412	Total	C	N	O	S	0	0	0
			3110	1971	512	617	10			
1	N	413	Total	C	N	O	S	0	0	0
			3109	1970	513	616	10			
1	O	412	Total	C	N	O	S	0	0	0
			3109	1970	512	617	10			
1	P	417	Total	C	N	O	S	0	0	0
			3138	1989	517	622	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	417	Total	C	N	O	S	0	0	0
			3138	1989	517	622	10			
1	R	411	Total	C	N	O	S	0	0	0
			3101	1966	511	614	10			
1	S	414	Total	C	N	O	S	0	0	0
			3116	1975	514	617	10			
1	T	418	Total	C	N	O	S	0	0	0
			3150	1998	518	624	10			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
A	330	SER	MET	ENGINEERED	UNP Q6S9I7
A	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
A	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
A	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
B	330	SER	MET	ENGINEERED	UNP Q6S9I7
B	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
B	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
B	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
C	330	SER	MET	ENGINEERED	UNP Q6S9I7
C	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
C	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
C	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
D	330	SER	MET	ENGINEERED	UNP Q6S9I7
D	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
D	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
D	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
E	330	SER	MET	ENGINEERED	UNP Q6S9I7
E	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
E	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
E	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
F	330	SER	MET	ENGINEERED	UNP Q6S9I7
F	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
F	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
F	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
G	330	SER	MET	ENGINEERED	UNP Q6S9I7
G	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
G	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
G	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
H	330	SER	MET	ENGINEERED	UNP Q6S9I7
H	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
H	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
H	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	135	GLU	ASP	ENGINEERED	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	330	SER	MET	ENGINEERED	UNP Q6S9I7
I	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
I	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
I	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
J	330	SER	MET	ENGINEERED	UNP Q6S9I7
J	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
J	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
J	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
K	330	SER	MET	ENGINEERED	UNP Q6S9I7
K	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
K	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
K	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
L	330	SER	MET	ENGINEERED	UNP Q6S9I7
L	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
L	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
L	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
M	330	SER	MET	ENGINEERED	UNP Q6S9I7
M	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
M	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
M	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
N	330	SER	MET	ENGINEERED	UNP Q6S9I7
N	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
N	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
N	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
O	330	SER	MET	ENGINEERED	UNP Q6S9I7
O	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
O	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
O	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
P	330	SER	MET	ENGINEERED	UNP Q6S9I7
P	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
P	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
P	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
Q	330	SER	MET	ENGINEERED	UNP Q6S9I7
Q	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
Q	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
Q	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
R	330	SER	MET	ENGINEERED	UNP Q6S9I7
R	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
R	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
R	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
S	330	SER	MET	ENGINEERED	UNP Q6S9I7
S	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
S	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
S	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	135	GLU	ASP	ENGINEERED	UNP Q6S9I7
T	330	SER	MET	ENGINEERED	UNP Q6S9I7
T	331	GLY	TRP	ENGINEERED	UNP Q6S9I7
T	453	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	454	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	455	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	456	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	457	HIS	-	EXPRESSION TAG	UNP Q6S9I7
T	458	HIS	-	EXPRESSION TAG	UNP Q6S9I7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	R	1	Total Cl 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	R	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	252	Total 252	O 252	0	0
4	B	250	Total 250	O 250	0	0
4	C	204	Total 204	O 204	0	0
4	D	245	Total 245	O 245	0	0
4	E	211	Total 211	O 211	0	0
4	F	235	Total 235	O 235	0	0
4	G	226	Total 226	O 226	0	0
4	H	195	Total 195	O 195	0	0
4	I	202	Total 202	O 202	0	0
4	J	213	Total 213	O 213	0	0
4	K	226	Total 226	O 226	0	0

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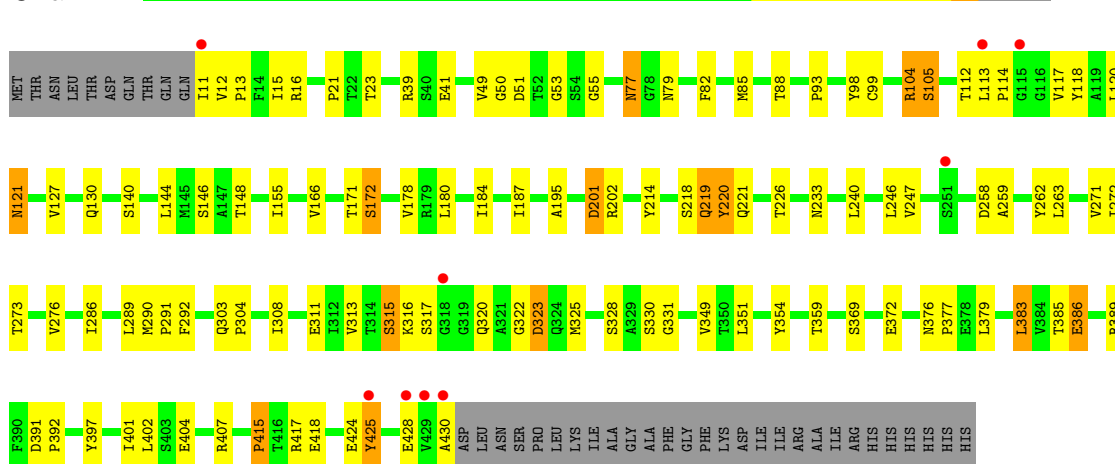
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	234	Total 234	O 234	0	0
4	M	235	Total 235	O 235	0	0
4	N	195	Total 195	O 195	0	0
4	O	216	Total 216	O 216	0	0
4	P	183	Total 183	O 183	0	0
4	Q	201	Total 201	O 201	0	0
4	R	226	Total 226	O 226	0	0
4	S	226	Total 226	O 226	0	0
4	T	270	Total 270	O 270	0	0

### 3 Residue-property plots

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.

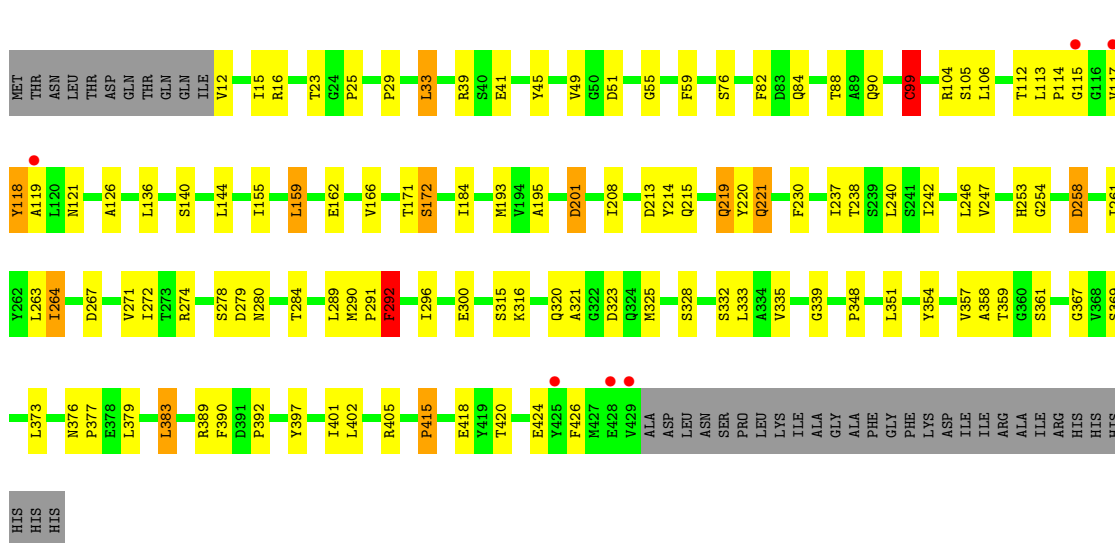
#### • Molecule 1: structural polypeptide VP2

Chain A:



#### • Molecule 1: structural polypeptide VP2

Chain B:



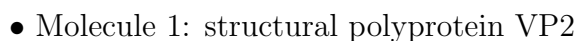
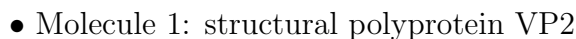
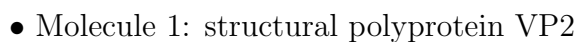
#### • Molecule 1: structural polypeptide VP2

Chain C:

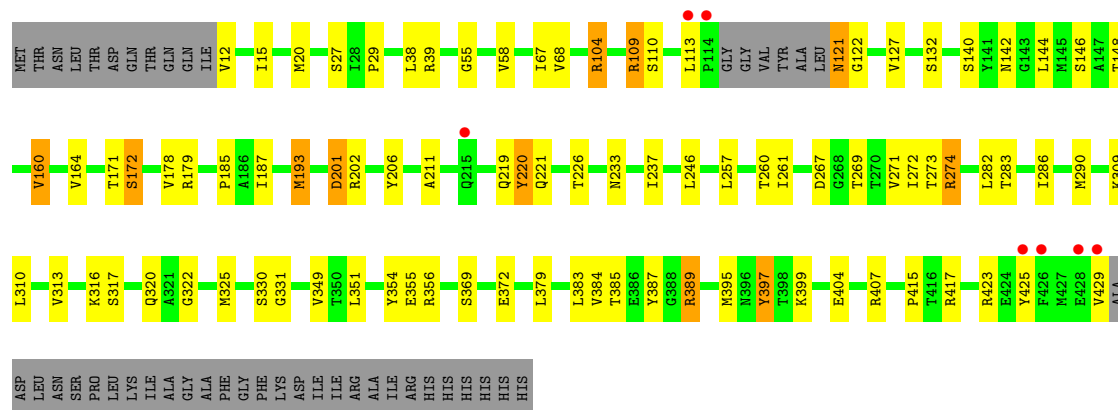






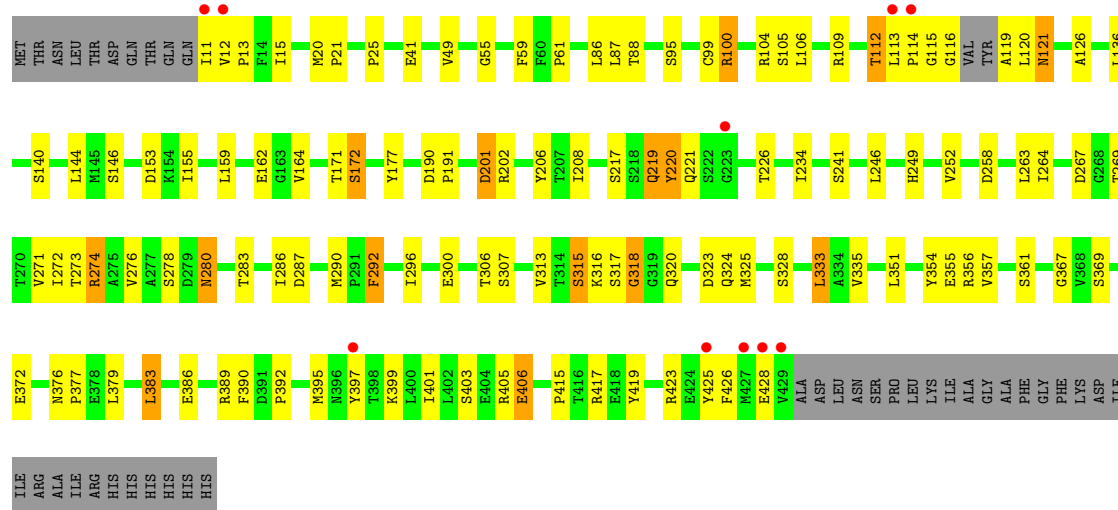






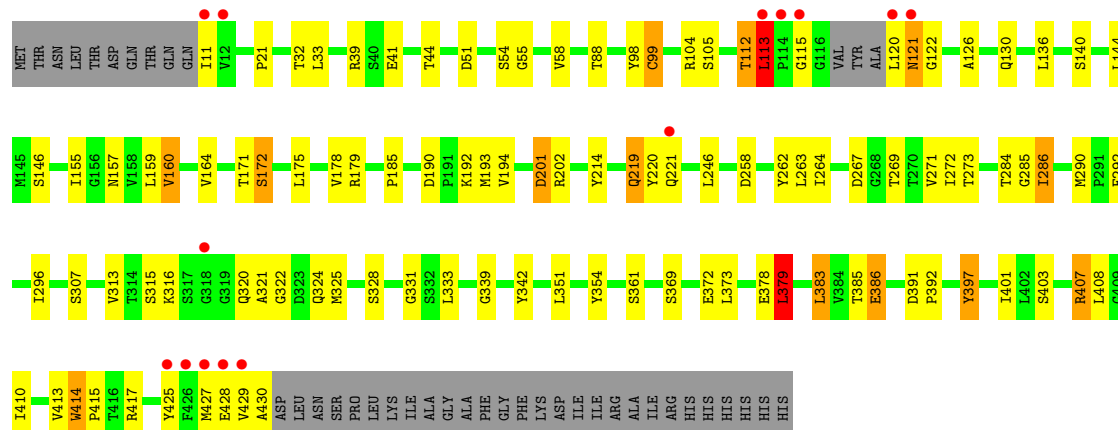
• Molecule 1: structural polypeptide VP2

Chain P:



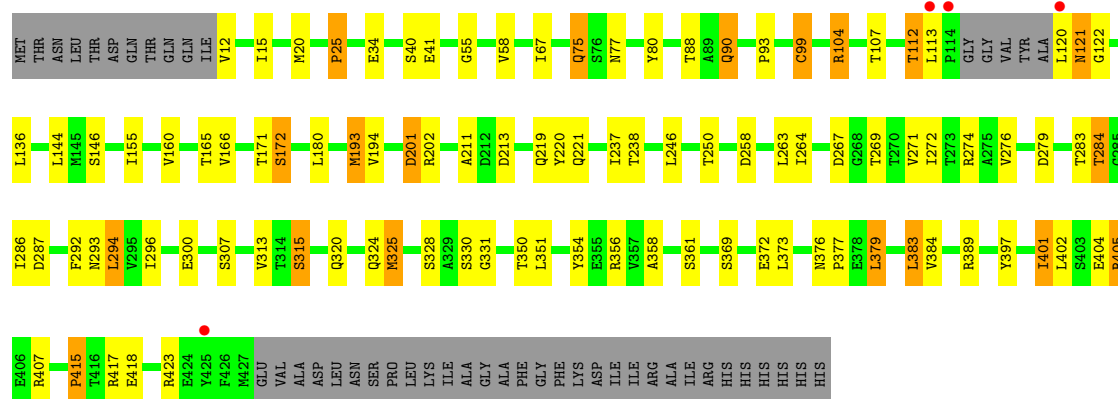
• Molecule 1: structural polypeptide VP2

Chain Q:



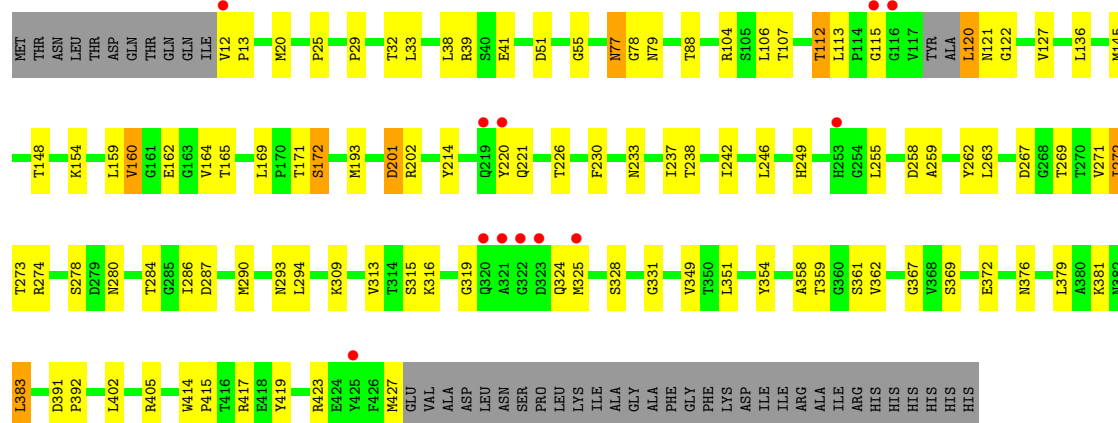
• Molecule 1: structural polypeptide VP2

Chain R:



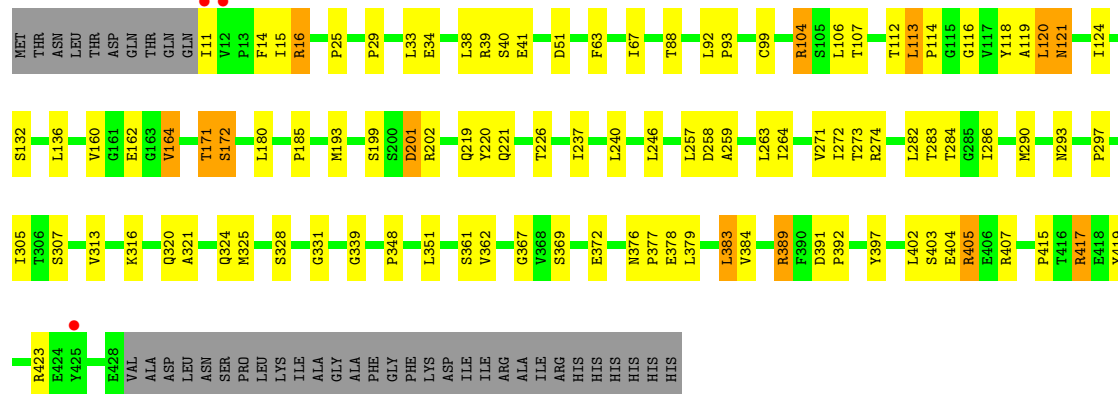
• Molecule 1: structural polypeptide VP2

Chain S:



• Molecule 1: structural polypeptide VP2

Chain T:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	316.41Å 316.41Å 316.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 49.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.6 (40.00-2.60) 89.6 (49.42-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.165 , 0.215 0.166 , 0.215	Depositor DCC
$R_{free}$ test set	14255 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 286972 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	66956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.81	1/3226 (0.0%)	0.90	4/4407 (0.1%)
1	B	0.87	2/3213 (0.1%)	0.96	3/4389 (0.1%)
1	C	0.77	0/3180	0.92	5/4342 (0.1%)
1	D	0.81	0/3179	0.94	8/4340 (0.2%)
1	E	0.82	2/3192 (0.1%)	0.94	3/4359 (0.1%)
1	F	0.79	0/3175	0.92	5/4335 (0.1%)
1	G	0.80	1/3172 (0.0%)	0.91	3/4331 (0.1%)
1	H	0.75	0/3179	0.88	5/4341 (0.1%)
1	I	0.74	1/3180 (0.0%)	0.88	3/4342 (0.1%)
1	J	0.76	0/3163	0.88	2/4318 (0.0%)
1	K	0.76	1/3199 (0.0%)	0.89	2/4368 (0.0%)
1	L	0.79	0/3214	0.90	4/4390 (0.1%)
1	M	0.77	0/3172	0.89	3/4331 (0.1%)
1	N	0.79	0/3171	0.91	5/4329 (0.1%)
1	O	0.75	0/3171	0.90	4/4330 (0.1%)
1	P	0.79	0/3200	0.94	2/4369 (0.0%)
1	Q	0.75	1/3200 (0.0%)	0.89	4/4369 (0.1%)
1	R	0.80	0/3163	0.94	4/4319 (0.1%)
1	S	0.79	0/3178	0.92	3/4339 (0.1%)
1	T	0.83	2/3214 (0.1%)	0.93	4/4390 (0.1%)
All	All	0.79	11/63741 (0.0%)	0.91	76/87038 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
1	L	0	1
1	O	0	3
1	Q	0	1
All	All	0	11

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	PHE	CB-CG	-8.56	1.36	1.51
1	E	327	TRP	CB-CG	6.17	1.61	1.50
1	T	378	GLU	CG-CD	6.11	1.61	1.51
1	K	99	CYS	CB-SG	-5.85	1.72	1.81
1	G	99	CYS	CB-SG	-5.50	1.72	1.81

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	120	LEU	CA-CB-CG	7.95	133.57	115.30
1	G	415	PRO	N-CA-C	-7.75	91.94	112.10
1	S	415	PRO	N-CA-C	-7.72	92.03	112.10
1	Q	415	PRO	N-CA-C	-7.60	92.33	112.10
1	K	415	PRO	N-CA-C	-7.60	92.35	112.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	TYR	Sidechain
1	D	206	TYR	Sidechain
1	D	397	TYR	Sidechain
1	D	45	TYR	Sidechain
1	J	397	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3162	0	3141	111	0
1	B	3149	0	3125	102	0
1	C	3118	0	3097	92	0
1	D	3118	0	3099	62	0
1	E	3130	0	3111	99	0
1	F	3113	0	3094	85	0
1	G	3110	0	3086	111	0
1	H	3117	0	3095	84	0
1	I	3118	0	3097	69	0
1	J	3102	0	3077	89	0
1	K	3137	0	3115	94	0
1	L	3150	0	3127	95	0
1	M	3110	0	3086	88	0
1	N	3109	0	3086	83	0
1	O	3109	0	3084	79	0
1	P	3138	0	3117	102	0
1	Q	3138	0	3117	95	0
1	R	3101	0	3080	107	0
1	S	3116	0	3095	92	0
1	T	3150	0	3127	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	P	1	0	0	0	0
2	R	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
4	A	252	0	0	1	0
4	B	250	0	0	2	0
4	C	204	0	0	3	0
4	D	245	0	0	5	0
4	E	211	0	0	0	0
4	F	235	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	226	0	0	14	0
4	H	195	0	0	7	0
4	I	202	0	0	2	0
4	J	213	0	0	7	0
4	K	226	0	0	10	0
4	L	234	0	0	2	0
4	M	235	0	0	4	0
4	N	195	0	0	4	0
4	O	216	0	0	6	0
4	P	183	0	0	4	0
4	Q	201	0	0	1	0
4	R	226	0	0	4	0
4	S	226	0	0	8	0
4	T	270	0	0	5	0
All	All	66956	0	62056	1715	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 1715 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:J:512:HOH:O	1:P:121:ASN:HB3	1.32	1.23
1:T:417:ARG:HH11	1:T:417:ARG:HB2	1.07	1.15
1:R:379:LEU:HD23	1:R:383:LEU:HD22	1.28	1.14
1:G:279:ASP:HB3	1:K:286:ILE:HD11	1.31	1.12
1:D:379:LEU:HG	1:D:383:LEU:HD12	1.27	1.10

There are no symmetry-related clashes.

## 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	418/458 (91%)	397 (95%)	18 (4%)	3 (1%)	30 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	416/458 (91%)	399 (96%)	16 (4%)	1 (0%)	56	82
1	C	409/458 (89%)	390 (95%)	17 (4%)	2 (0%)	38	67
1	D	409/458 (89%)	387 (95%)	21 (5%)	1 (0%)	56	82
1	E	411/458 (90%)	392 (95%)	18 (4%)	1 (0%)	56	82
1	F	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	30	58
1	G	408/458 (89%)	389 (95%)	17 (4%)	2 (0%)	38	67
1	H	409/458 (89%)	390 (95%)	18 (4%)	1 (0%)	56	82
1	I	409/458 (89%)	388 (95%)	20 (5%)	1 (0%)	56	82
1	J	407/458 (89%)	387 (95%)	17 (4%)	3 (1%)	30	58
1	K	413/458 (90%)	391 (95%)	20 (5%)	2 (0%)	38	67
1	L	416/458 (91%)	396 (95%)	17 (4%)	3 (1%)	30	58
1	M	408/458 (89%)	388 (95%)	19 (5%)	1 (0%)	56	82
1	N	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	30	58
1	O	408/458 (89%)	386 (95%)	19 (5%)	3 (1%)	30	58
1	P	413/458 (90%)	388 (94%)	21 (5%)	4 (1%)	22	45
1	Q	413/458 (90%)	394 (95%)	17 (4%)	2 (0%)	38	67
1	R	407/458 (89%)	391 (96%)	15 (4%)	1 (0%)	56	82
1	S	410/458 (90%)	389 (95%)	19 (5%)	2 (0%)	38	67
1	T	416/458 (91%)	392 (94%)	23 (6%)	1 (0%)	56	82
All	All	8218/9160 (90%)	7810 (95%)	368 (4%)	40 (0%)	38	67

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	115	GLY
1	Q	115	GLY
1	A	220	TYR
1	G	321	ALA
1	J	220	TYR

### 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	352/385 (91%)	336 (96%)	16 (4%)	38	67
1	B	351/385 (91%)	330 (94%)	21 (6%)	27	51
1	C	349/385 (91%)	332 (95%)	17 (5%)	35	62
1	D	349/385 (91%)	334 (96%)	15 (4%)	40	69
1	E	350/385 (91%)	332 (95%)	18 (5%)	33	60
1	F	348/385 (90%)	330 (95%)	18 (5%)	32	59
1	G	348/385 (90%)	328 (94%)	20 (6%)	29	54
1	H	349/385 (91%)	332 (95%)	17 (5%)	35	62
1	I	349/385 (91%)	336 (96%)	13 (4%)	45	75
1	J	347/385 (90%)	327 (94%)	20 (6%)	28	53
1	K	350/385 (91%)	324 (93%)	26 (7%)	20	38
1	L	351/385 (91%)	326 (93%)	25 (7%)	21	40
1	M	348/385 (90%)	328 (94%)	20 (6%)	29	54
1	N	347/385 (90%)	327 (94%)	20 (6%)	28	53
1	O	348/385 (90%)	335 (96%)	13 (4%)	45	75
1	P	350/385 (91%)	324 (93%)	26 (7%)	20	38
1	Q	350/385 (91%)	331 (95%)	19 (5%)	31	57
1	R	347/385 (90%)	328 (94%)	19 (6%)	30	56
1	S	348/385 (90%)	334 (96%)	14 (4%)	42	73
1	T	351/385 (91%)	329 (94%)	22 (6%)	25	49
All	All	6982/7700 (91%)	6603 (95%)	379 (5%)	31	57

5 of 379 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	407	ARG
1	L	202	ARG
1	S	201	ASP
1	K	51	ASP
1	K	379	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	130	GLN
1	L	233	ASN
1	S	293	ASN
1	J	233	ASN
1	K	233	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	420/458 (91%)	-0.53	9 (2%) 60 58	23, 33, 72, 105	0
1	B	418/458 (91%)	-0.64	6 (1%) 72 72	20, 32, 67, 106	0
1	C	413/458 (90%)	-0.49	11 (2%) 52 49	26, 37, 72, 105	0
1	D	413/458 (90%)	-0.49	7 (1%) 67 66	23, 34, 63, 106	0
1	E	415/458 (90%)	-0.38	10 (2%) 56 53	27, 36, 74, 114	0
1	F	413/458 (90%)	-0.58	6 (1%) 70 71	22, 35, 66, 98	0
1	G	412/458 (89%)	-0.61	5 (1%) 75 77	25, 37, 61, 106	0
1	H	413/458 (90%)	-0.46	11 (2%) 52 49	27, 39, 67, 114	0
1	I	413/458 (90%)	-0.40	12 (2%) 49 46	28, 38, 71, 107	0
1	J	411/458 (89%)	-0.49	6 (1%) 70 71	27, 38, 70, 99	0
1	K	417/458 (91%)	-0.44	9 (2%) 59 56	27, 38, 74, 108	0
1	L	418/458 (91%)	-0.38	9 (2%) 59 56	24, 34, 73, 103	0
1	M	412/458 (89%)	-0.38	18 (4%) 33 29	25, 38, 68, 105	0
1	N	413/458 (90%)	-0.50	6 (1%) 70 71	27, 38, 68, 104	0
1	O	412/458 (89%)	-0.54	7 (1%) 67 66	27, 37, 72, 104	0
1	P	417/458 (91%)	-0.53	10 (2%) 56 53	27, 39, 82, 112	0
1	Q	417/458 (91%)	-0.40	14 (3%) 43 39	27, 39, 77, 118	0
1	R	411/458 (89%)	-0.61	4 (0%) 79 81	26, 36, 56, 102	0
1	S	414/458 (90%)	-0.42	12 (2%) 49 46	25, 35, 65, 95	0
1	T	418/458 (91%)	-0.70	3 (0%) 84 86	23, 33, 62, 101	0
All	All	8290/9160 (90%)	-0.50	175 (2%) 60 58	20, 37, 70, 118	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	113	LEU	5.3
1	P	223	GLY	5.0
1	E	425	TYR	5.0
1	Q	113	LEU	5.0
1	H	425	TYR	4.9

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	B	5501	1/1	0.14	1.44	26,26,26,26	1
2	CL	I	5507	1/1	0.19	0.43	33,33,33,33	0
2	CL	A	5503	1/1	0.20	0.33	32,32,32,32	0
2	CL	C	5504	1/1	0.19	0.03	30,30,30,30	0
2	CL	R	5508	1/1	0.14	-0.05	27,27,27,27	0
2	CL	G	5505	1/1	0.18	-0.19	33,33,33,33	0
2	CL	H	5506	1/1	0.12	-1.21	31,31,31,31	0
2	CL	P	5502	1/1	0.10	-2.62	26,26,26,26	1
3	CA	G	5905	1/1	0.02	-4.43	45,45,45,45	0
3	CA	H	5906	1/1	0.03	-4.50	39,39,39,39	0
3	CA	R	5908	1/1	0.03	-4.51	36,36,36,36	0
3	CA	B	5901	1/1	0.03	-4.85	33,33,33,33	1
3	CA	C	5904	1/1	0.03	-4.92	39,39,39,39	0
3	CA	I	5907	1/1	0.02	-5.63	41,41,41,41	0
3	CA	A	5903	1/1	0.04	-5.92	34,34,34,34	0
3	CA	P	5902	1/1	0.03	-21.33	40,40,40,40	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.