



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:41 PM UTC

PDB ID : 3KZ4 / pdb_00003kz4
Title : Crystal Structure of the Rotavirus Double Layered Particle
Authors : McClain, B.; Settembre, E.C.; Bellamy, A.R.; Harrison, S.C.
Deposited on : 2009-12-07
Resolution : 3.80 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
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

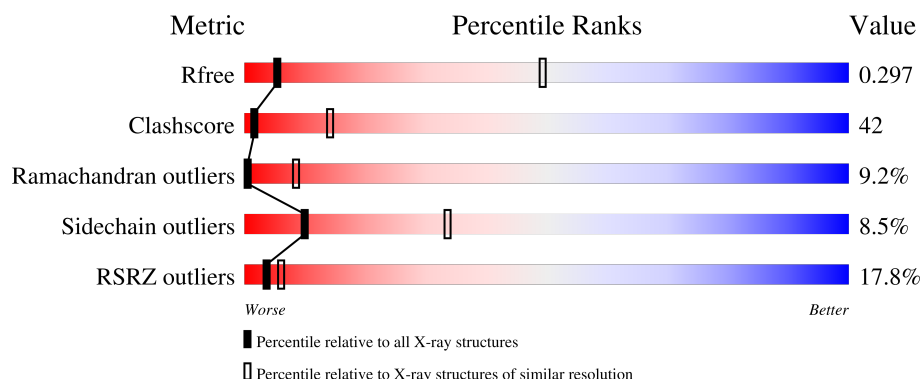
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



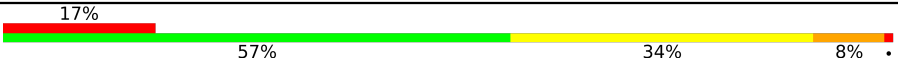
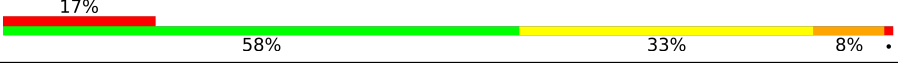
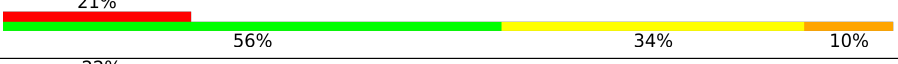
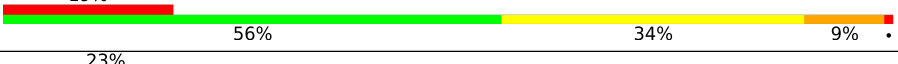
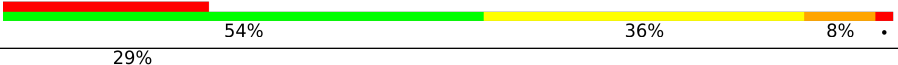
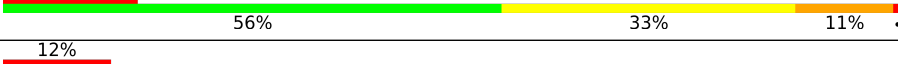
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	880	11% 14% 47% 24% 11%
1	B	880	7% 16% 47% 26% 8%
2	C	397	15% 59% 31% 9%
2	D	397	21% 55% 34% 11%
2	E	397	22% 56% 33% 9%

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Mol	Chain	Length	Quality of chain
2	F	397	
2	G	397	
2	H	397	
2	I	397	
2	J	397	
2	K	397	
2	L	397	
2	M	397	
2	N	397	
2	O	397	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 54109 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6374	4049	1099	1190	36			
1	B	810	Total	C	N	O	S	0	0	0
			6624	4211	1138	1239	36			

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	D	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	E	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	F	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	G	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	H	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	I	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	J	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	K	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	L	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	M	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	N	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

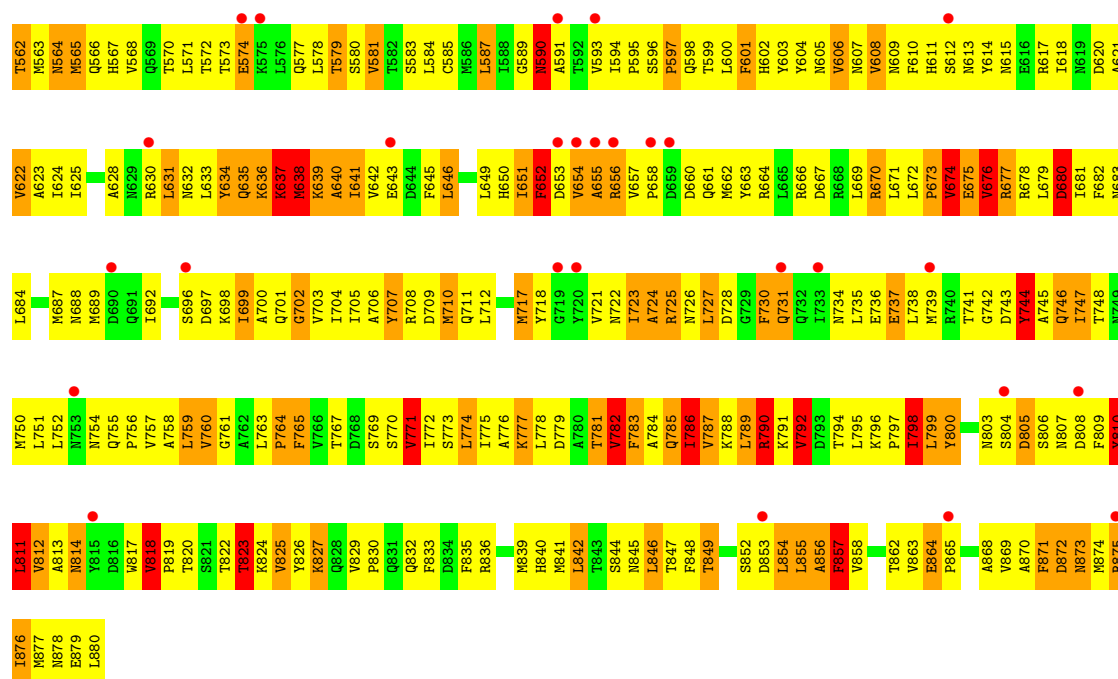
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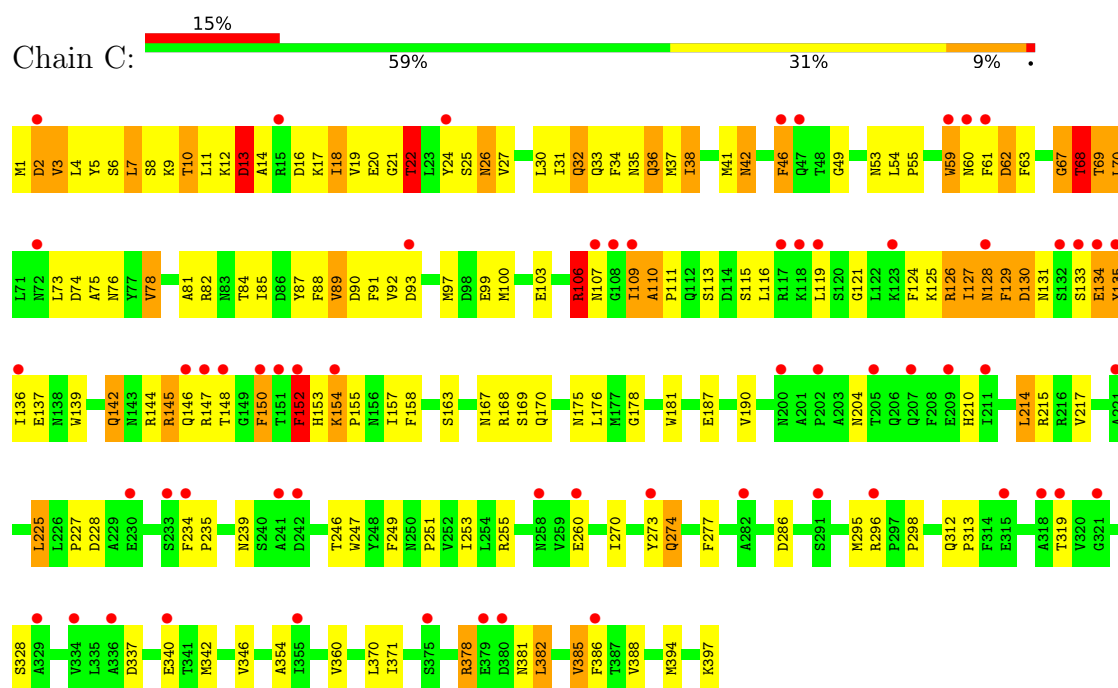
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

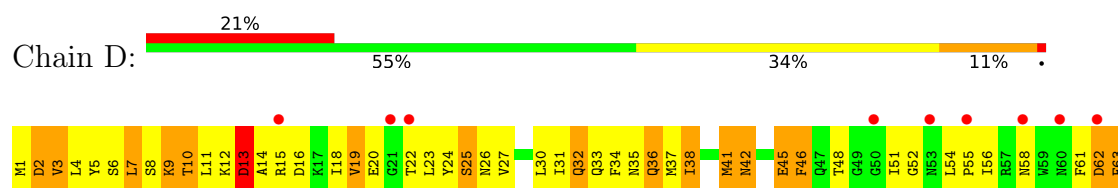
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	O	1	Total	Zn	0	0
			1	1		

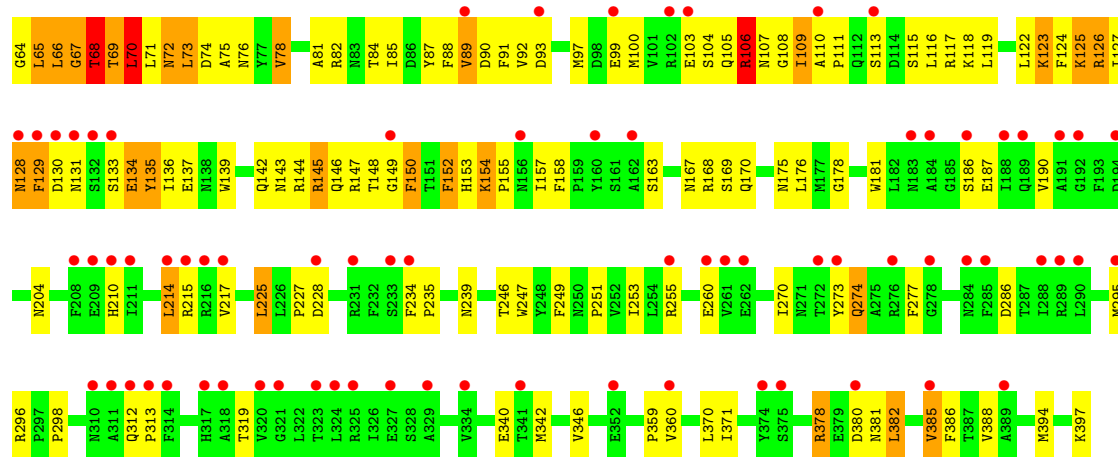


- Molecule 2: Intermediate capsid protein VP6

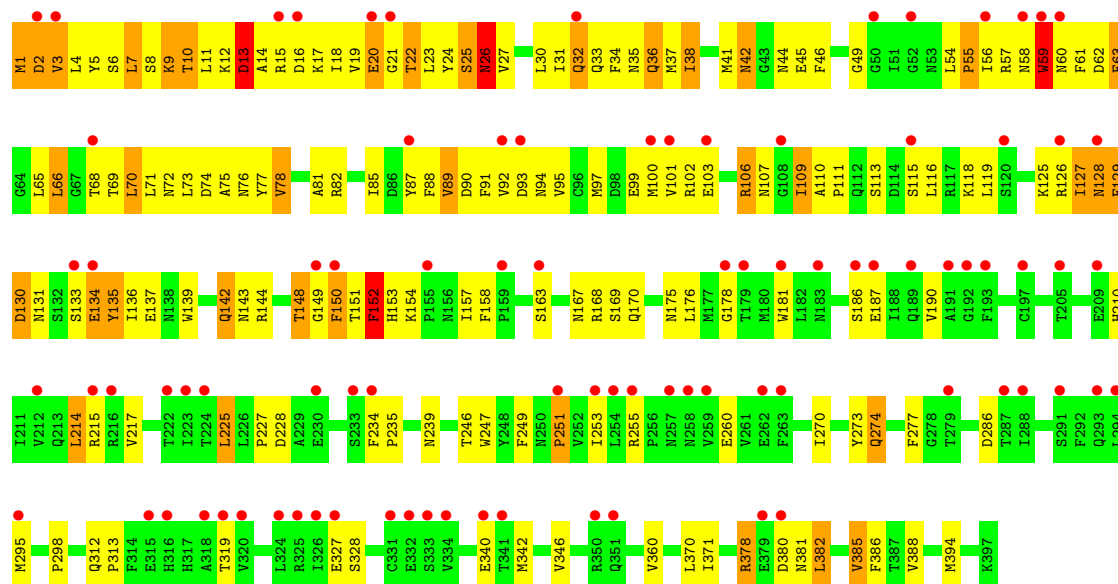


- Molecule 2: Intermediate capsid protein VP6

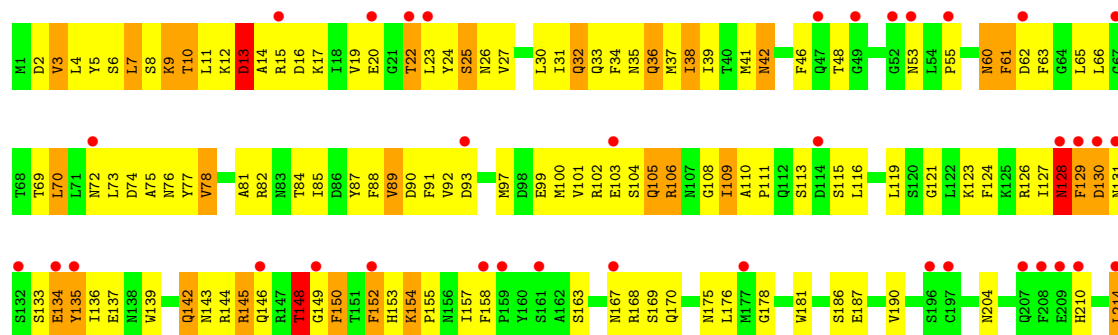


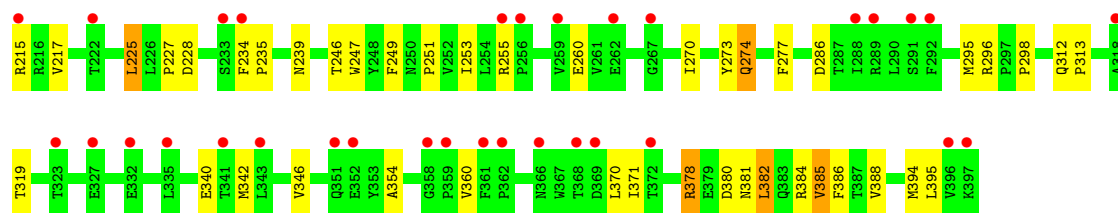


• Molecule 2: Intermediate capsid protein VP6

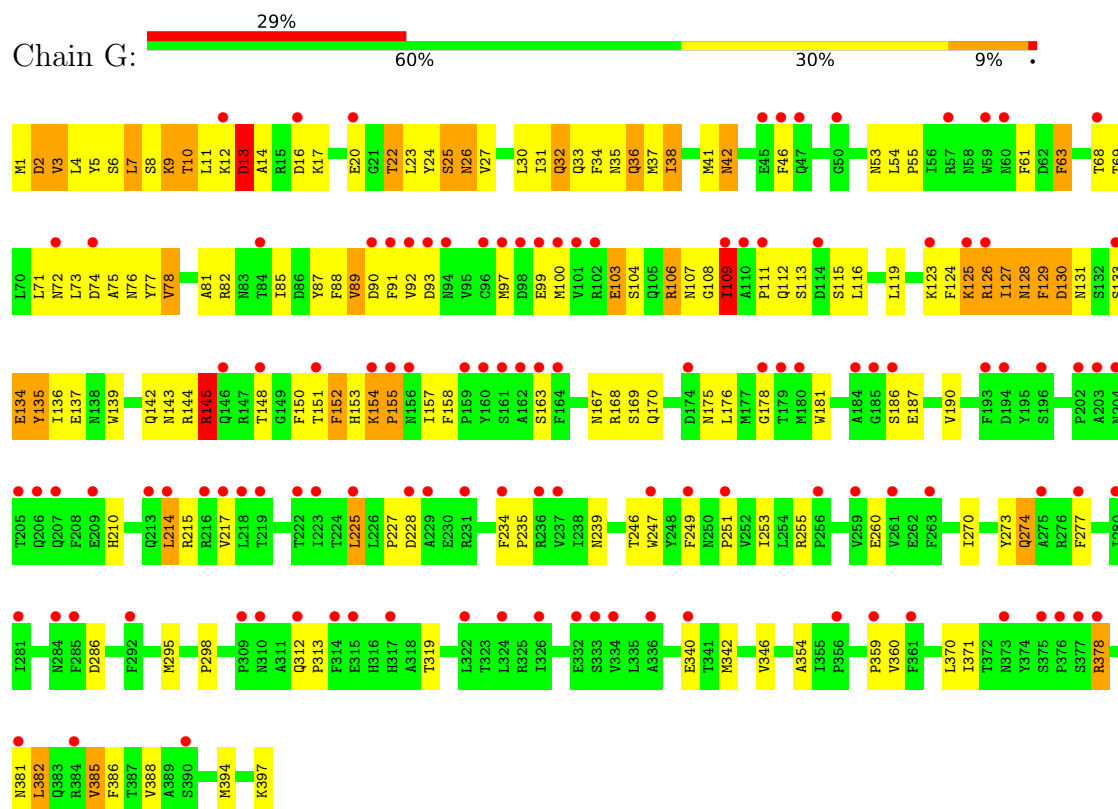


• Molecule 2: Intermediate capsid protein VP6

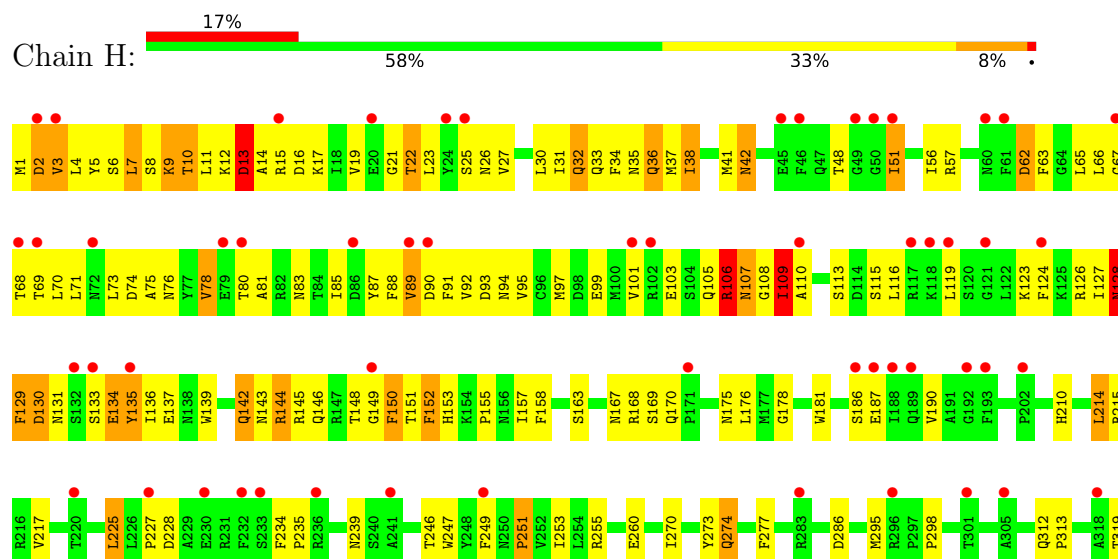




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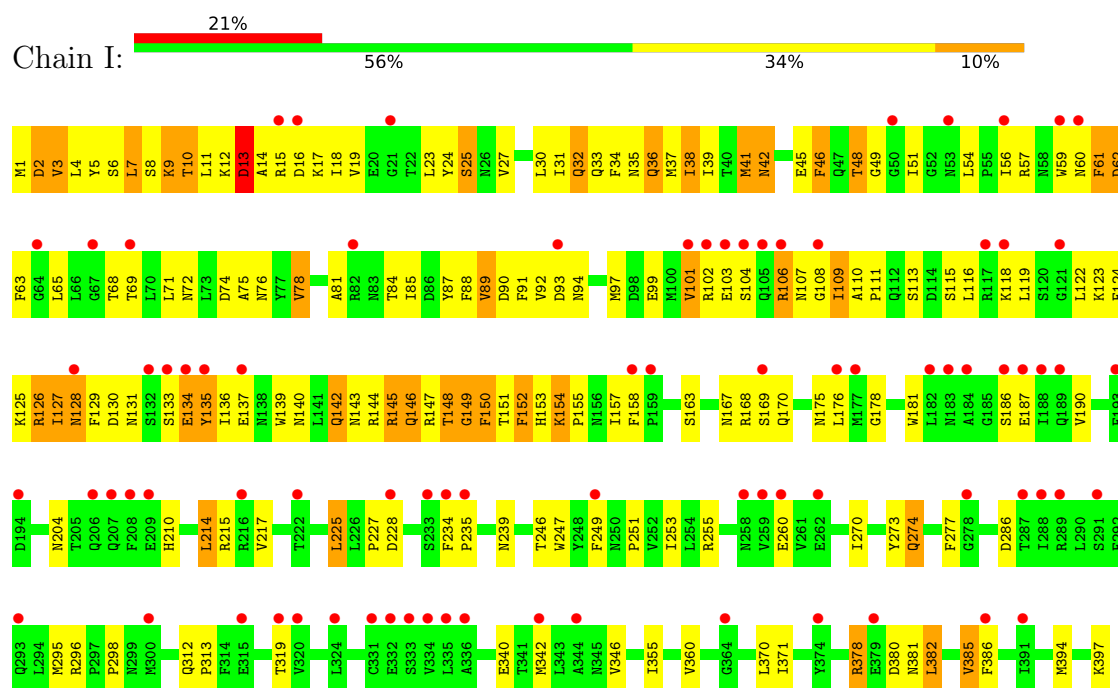


• Molecule 2: Intermediate capsid protein VP6

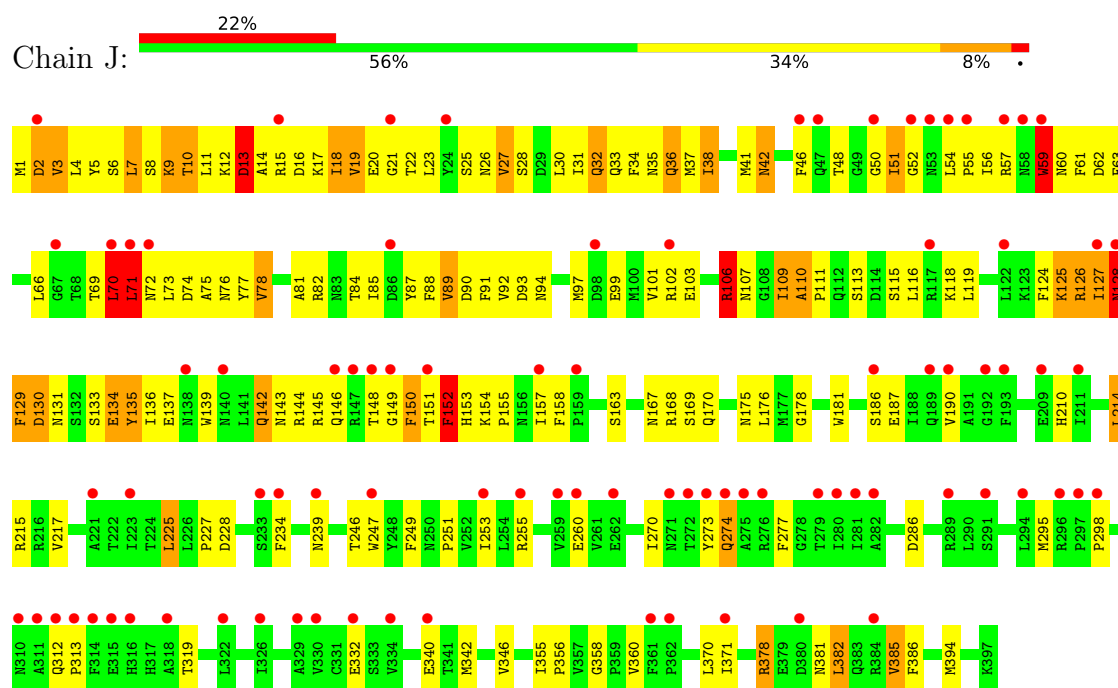




• Molecule 2: Intermediate capsid protein VP6

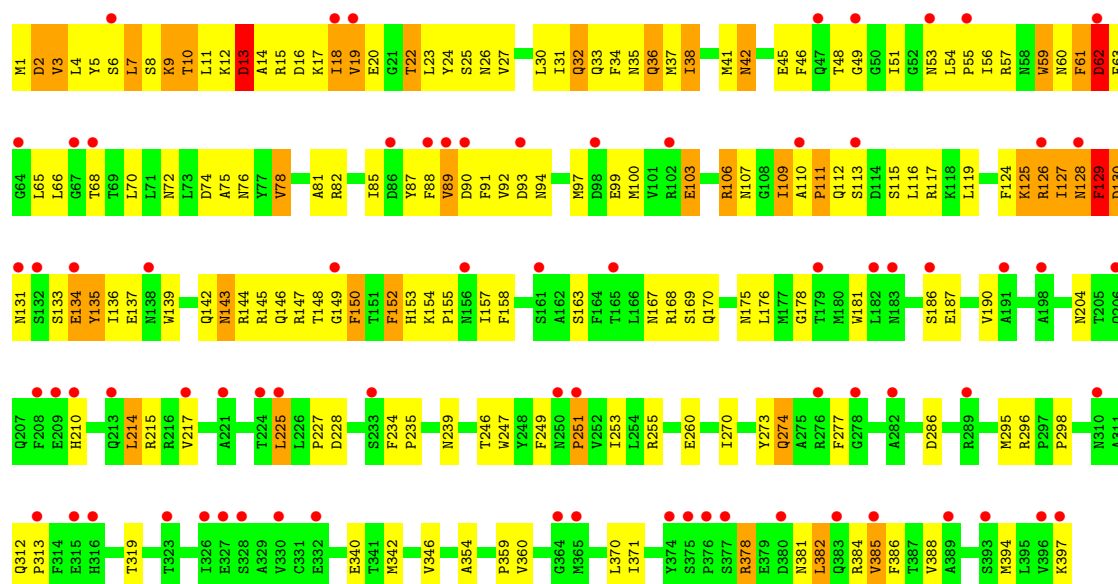


• Molecule 2: Intermediate capsid protein VP6

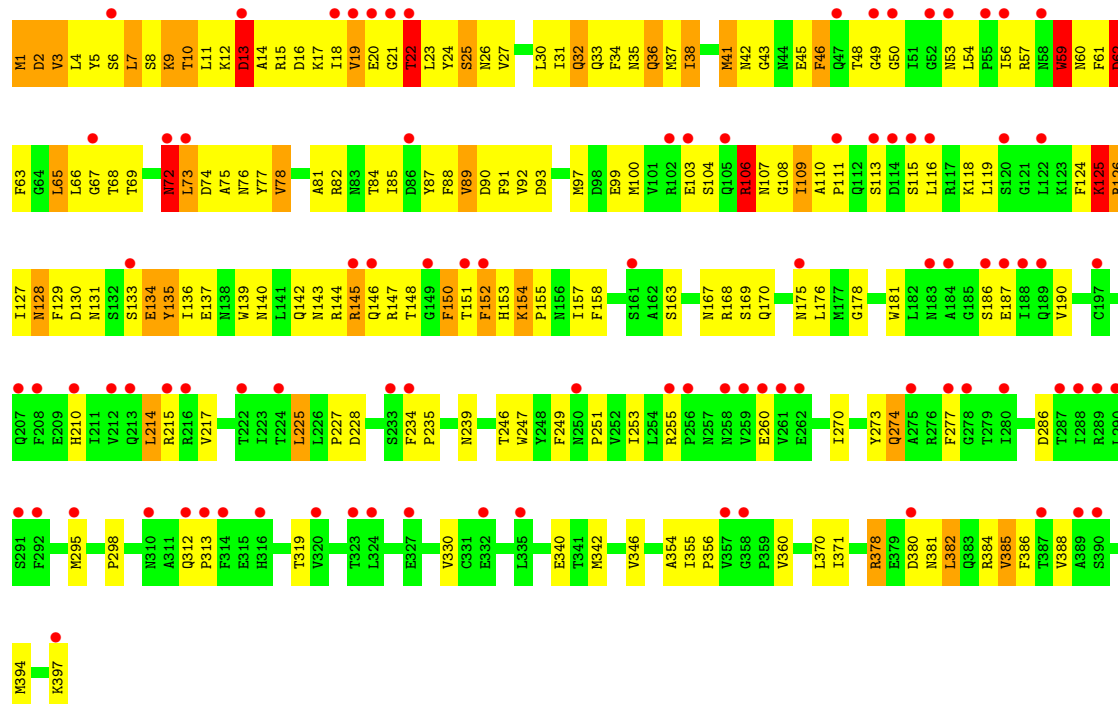


• Molecule 2: Intermediate capsid protein VP6

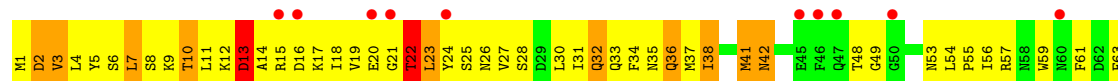


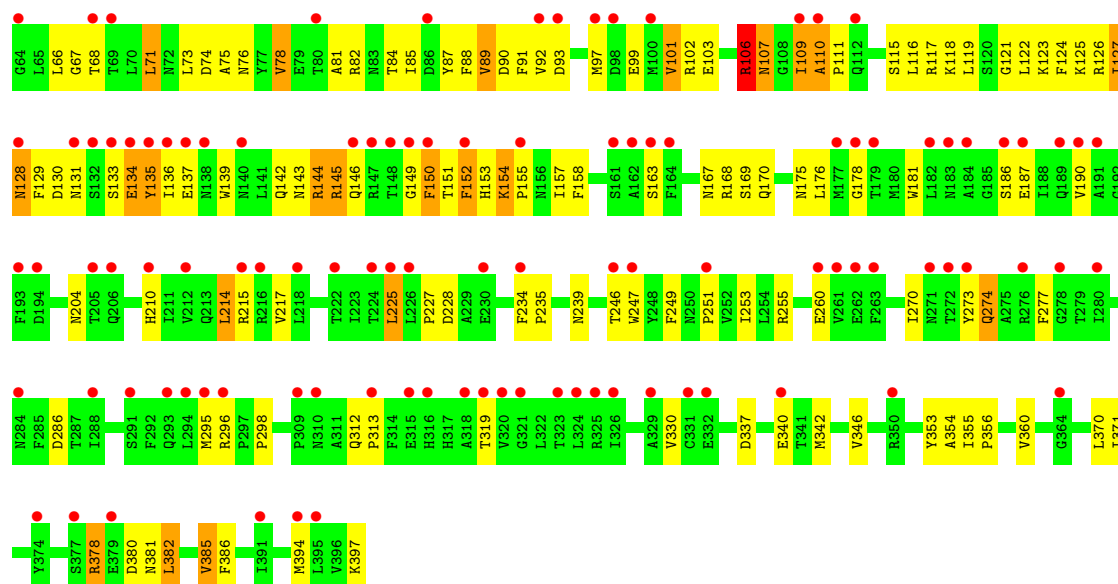


• Molecule 2: Intermediate capsid protein VP6

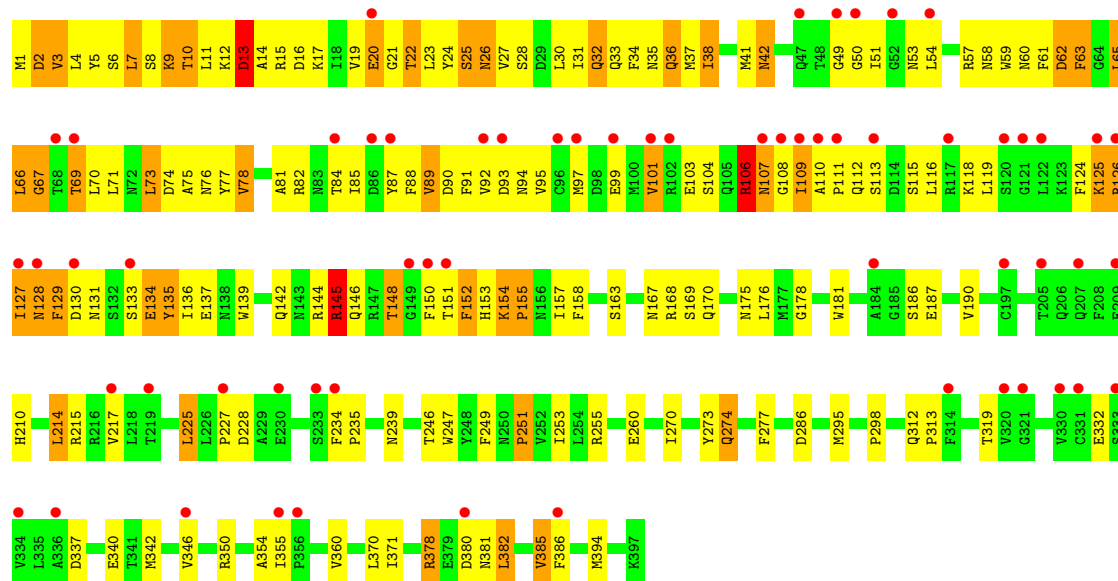


• Molecule 2: Intermediate capsid protein VP6

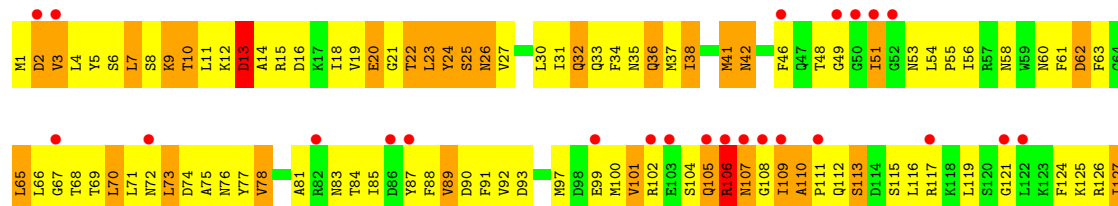


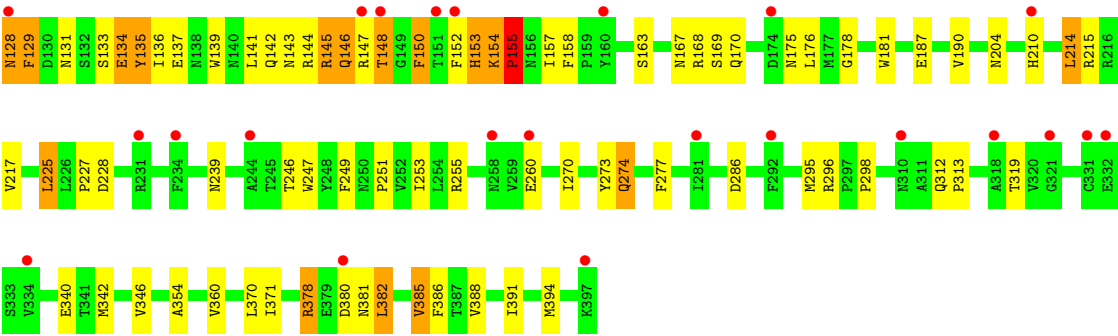


• Molecule 2: Intermediate capsid protein VP6



• Molecule 2: Intermediate capsid protein VP6





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	15.9 (30.00-3.80) 15.9 (30.00-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.328 , 0.339 0.290 , 0.297	Depositor DCC
R_{free} test set	47880 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	167.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	54109	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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:
ZN

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	0.56	0/6491	1.23	83/8806 (0.9%)
1	B	0.58	0/6745	1.21	75/9149 (0.8%)
2	C	0.62	1/3232 (0.0%)	1.05	17/4397 (0.4%)
2	D	0.63	1/3232 (0.0%)	1.03	12/4397 (0.3%)
2	E	0.62	1/3232 (0.0%)	1.04	16/4397 (0.4%)
2	F	0.62	1/3232 (0.0%)	1.02	11/4397 (0.3%)
2	G	0.61	1/3232 (0.0%)	1.03	13/4397 (0.3%)
2	H	0.62	1/3232 (0.0%)	1.00	10/4397 (0.2%)
2	I	0.63	1/3232 (0.0%)	1.03	13/4397 (0.3%)
2	J	0.62	1/3232 (0.0%)	1.04	17/4397 (0.4%)
2	K	0.63	2/3232 (0.1%)	1.03	16/4397 (0.4%)
2	L	0.62	1/3232 (0.0%)	1.03	15/4397 (0.3%)
2	M	0.63	1/3232 (0.0%)	1.05	13/4397 (0.3%)
2	N	0.62	1/3232 (0.0%)	1.03	13/4397 (0.3%)
2	O	0.64	2/3232 (0.1%)	1.08	19/4397 (0.4%)
All	All	0.61	15/55252 (0.0%)	1.08	343/75116 (0.5%)

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	A	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	247	TRP	NE1-CE2	-5.55	1.31	1.37
2	K	154	LYS	CA-CB	5.55	1.57	1.52
2	I	247	TRP	NE1-CE2	-5.51	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	247	TRP	NE1-CE2	-5.49	1.31	1.37
2	O	154	LYS	CA-CB	5.45	1.57	1.52

The worst 5 of 343 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	LEU	N-CA-C	-20.02	90.51	112.93
1	B	636	LYS	N-CA-C	-12.91	94.53	110.41
1	B	497	ILE	N-CA-C	-12.47	95.47	111.05
1	B	75	VAL	N-CA-C	-11.82	101.12	112.83
1	A	298	TYR	N-CA-C	11.39	131.01	114.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	6374	0	6394	1069	0
1	B	6624	0	6652	1209	0
2	C	3162	0	3101	185	0
2	D	3162	0	3101	195	0
2	E	3162	0	3101	181	0
2	F	3162	0	3101	174	0
2	G	3162	0	3101	160	0
2	H	3162	0	3101	189	0
2	I	3162	0	3101	230	0
2	J	3162	0	3101	203	0
2	K	3162	0	3101	182	0
2	L	3162	0	3101	192	0
2	M	3162	0	3101	190	0
2	N	3162	0	3101	205	0
2	O	3162	0	3101	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
All	All	54109	0	53359	4504	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 42.

The worst 5 of 4504 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:B:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:B:442:MET:HE1	1:B:463:ILE:HG12	1.29	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13
1:B:717:MET:HE1	1:B:830:PRO:HD2	1.25	1.13

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	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0	1
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	2
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	1	15
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	11
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	1	14
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	15
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	1	15
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	1	14
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	1	15
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	1	14
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	13
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	1	16
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	12
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	11
All	All	6722/6921 (97%)	5051 (75%)	1054 (16%)	617 (9%)	0	8

5 of 617 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	ALA

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	715/809 (88%)	604 (84%)	111 (16%)	2	15
1	B	744/809 (92%)	633 (85%)	111 (15%)	3	16
2	C	350/350 (100%)	326 (93%)	24 (7%)	14	40
2	D	350/350 (100%)	324 (93%)	26 (7%)	13	38
2	E	350/350 (100%)	327 (93%)	23 (7%)	15	41
2	F	350/350 (100%)	329 (94%)	21 (6%)	17	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	350/350 (100%)	329 (94%)	21 (6%)	17	43
2	H	350/350 (100%)	331 (95%)	19 (5%)	20	45
2	I	350/350 (100%)	330 (94%)	20 (6%)	18	44
2	J	350/350 (100%)	329 (94%)	21 (6%)	17	43
2	K	350/350 (100%)	330 (94%)	20 (6%)	18	44
2	L	350/350 (100%)	324 (93%)	26 (7%)	13	38
2	M	350/350 (100%)	325 (93%)	25 (7%)	13	39
2	N	350/350 (100%)	328 (94%)	22 (6%)	16	42
2	O	350/350 (100%)	329 (94%)	21 (6%)	17	43
All	All	6009/6168 (97%)	5498 (92%)	511 (8%)	10	33

5 of 511 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	128	ASN
2	M	2	ASP
2	E	170	GLN
2	L	274	GLN
2	N	103	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 261 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	35	ASN
2	N	142	GLN
2	O	284	ASN
2	D	128	ASN
2	C	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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.

No monomer is involved in short contacts.

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	781/880 (88%)	0.48	96 (12%) 8 12	62, 136, 196, 209	0
1	B	810/880 (92%)	0.35	61 (7%) 20 18	53, 131, 186, 209	0
2	C	397/397 (100%)	0.70	61 (15%) 5 8	81, 147, 203, 209	0
2	D	397/397 (100%)	0.97	83 (20%) 2 4	90, 154, 208, 209	0
2	E	397/397 (100%)	1.04	89 (22%) 2 4	72, 151, 201, 209	0
2	F	397/397 (100%)	0.82	69 (17%) 4 6	100, 182, 209, 209	0
2	G	397/397 (100%)	1.38	117 (29%) 1 2	82, 176, 209, 209	0
2	H	397/397 (100%)	0.89	69 (17%) 4 6	96, 174, 209, 209	0
2	I	397/397 (100%)	1.08	82 (20%) 2 4	83, 157, 208, 209	0
2	J	397/397 (100%)	1.14	88 (22%) 2 4	77, 155, 203, 209	0
2	K	397/397 (100%)	0.87	75 (18%) 3 5	79, 156, 208, 209	0
2	L	397/397 (100%)	1.08	92 (23%) 2 3	77, 150, 207, 209	0
2	M	397/397 (100%)	1.30	115 (28%) 1 2	81, 150, 208, 209	0
2	N	397/397 (100%)	0.71	61 (15%) 5 8	83, 150, 201, 209	0
2	O	397/397 (100%)	0.51	47 (11%) 9 12	75, 150, 200, 209	0
All	All	6752/6921 (97%)	0.83	1205 (17%) 4 6	53, 153, 208, 209	0

The worst 5 of 1205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	60	ASN	15.4
1	B	99	GLU	15.4
2	H	233	SER	13.1
2	G	110	ALA	12.7
2	D	55	PRO	12.3

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($\text{\AA}^2$)	Q<0.9
3	ZN	O	398	1/1	0.70	0.27	51,51,51,51	0
3	ZN	I	398	1/1	0.97	0.12	51,51,51,51	0
3	ZN	F	398	1/1	0.98	0.09	51,51,51,51	0
3	ZN	L	398	1/1	0.99	0.10	51,51,51,51	0
3	ZN	C	398	1/1	0.99	0.08	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.