



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3GZT
EMDB ID: : EMD-1571
Title : VP7 recoated rotavirus DLP
Authors : Chen, J.Z.; Settembre, E.C.; Harrison, S.C.; Grigorieff, N.
Deposited on : 2009-04-07
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

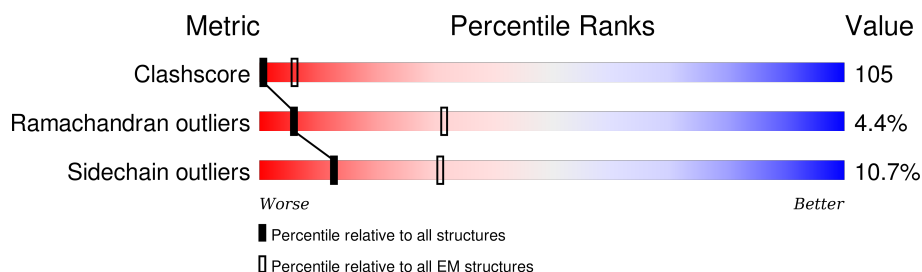
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	255	35% 48% 14% .
1	F	255	32% 50% 14% .
1	G	255	31% 50% 14% .
1	H	255	32% 50% 14% .
1	I	255	33% 50% 13% .
1	J	255	32% 51% 12% 5%
1	K	255	33% 51% 13% .
1	L	255	32% 51% 12% .
1	M	255	32% 50% 14% .

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Mol	Chain	Length	Quality of chain
1	N	255	<div><div></div><div>31%52%13%</div><div></div></div>
1	O	255	<div><div></div><div>33%49%14%</div><div></div></div>
1	P	255	<div><div></div><div>32%51%13%</div><div></div></div>
1	Q	255	<div><div></div><div>33%50%14%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26537 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	F	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	G	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	H	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	I	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	J	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	K	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	L	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	M	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	N	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	O	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	P	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
1	Q	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	171	THR	ALA	VARIANT	UNP P12476
F	171	THR	ALA	VARIANT	UNP P12476
G	171	THR	ALA	VARIANT	UNP P12476
H	171	THR	ALA	VARIANT	UNP P12476

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Chain	Residue	Modelled	Actual	Comment	Reference
I	171	THR	ALA	VARIANT	UNP P12476
J	171	THR	ALA	VARIANT	UNP P12476
K	171	THR	ALA	VARIANT	UNP P12476
L	171	THR	ALA	VARIANT	UNP P12476
M	171	THR	ALA	VARIANT	UNP P12476
N	171	THR	ALA	VARIANT	UNP P12476
O	171	THR	ALA	VARIANT	UNP P12476
P	171	THR	ALA	VARIANT	UNP P12476
Q	171	THR	ALA	VARIANT	UNP P12476

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	B	2	Total	C	N	O	0
			28	16	2	10	
2	G	2	Total	C	N	O	0
			28	16	2	10	
2	H	2	Total	C	N	O	0
			28	16	2	10	
2	F	2	Total	C	N	O	0
			28	16	2	10	
2	J	2	Total	C	N	O	0
			28	16	2	10	
2	K	2	Total	C	N	O	0
			28	16	2	10	
2	I	2	Total	C	N	O	0
			28	16	2	10	
2	M	2	Total	C	N	O	0
			28	16	2	10	
2	N	2	Total	C	N	O	0
			28	16	2	10	
2	L	2	Total	C	N	O	0
			28	16	2	10	
2	P	2	Total	C	N	O	0
			28	16	2	10	
2	Q	2	Total	C	N	O	0
			28	16	2	10	
2	O	2	Total	C	N	O	0
			28	16	2	10	

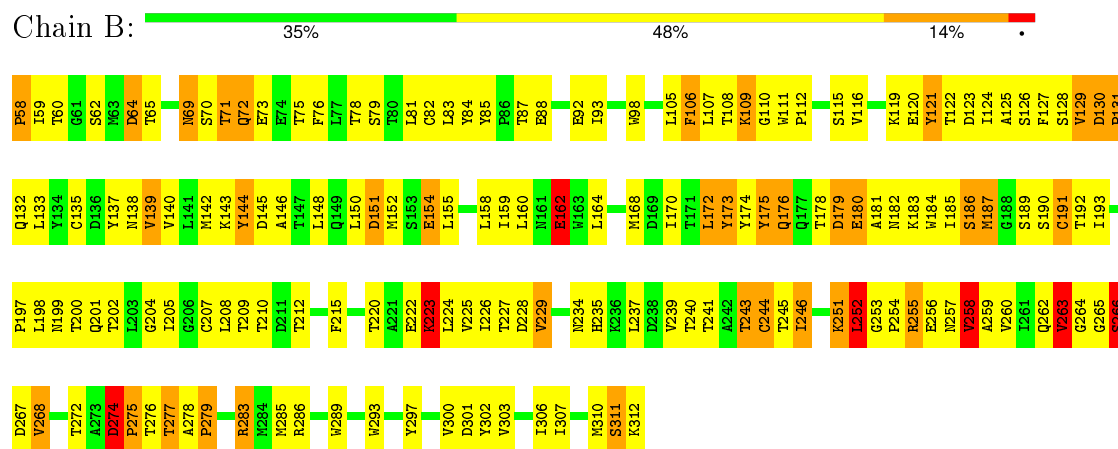
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	P	2	Total 2	Ca 2	0
3	G	2	Total 2	Ca 2	0
3	J	2	Total 2	Ca 2	0
3	Q	3	Total 3	Ca 3	0
3	K	2	Total 2	Ca 2	0
3	H	2	Total 2	Ca 2	0
3	B	4	Total 4	Ca 4	0
3	I	2	Total 2	Ca 2	0
3	N	2	Total 2	Ca 2	0
3	X	1	Total 1	Ca 1	0
3	O	2	Total 2	Ca 2	0
3	L	2	Total 2	Ca 2	0
3	F	2	Total 2	Ca 2	0
3	M	2	Total 2	Ca 2	0

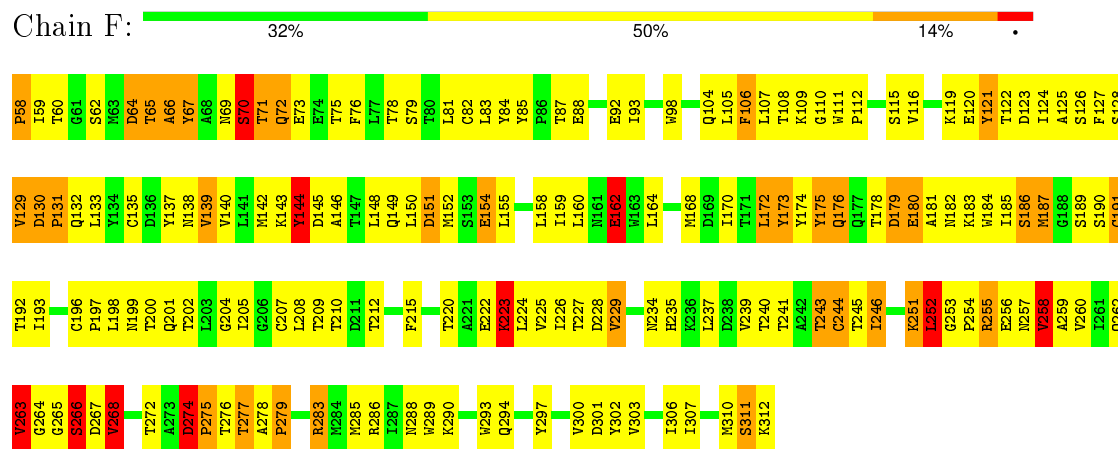
3 Residue-property plots

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. 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. 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.

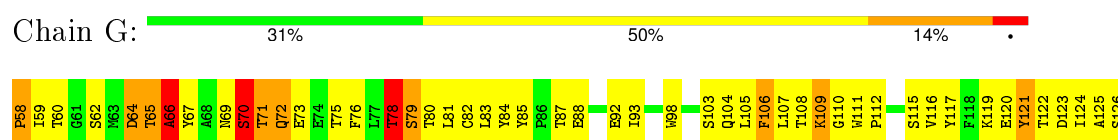
• Molecule 1: Outer capsid glycoprotein VP7

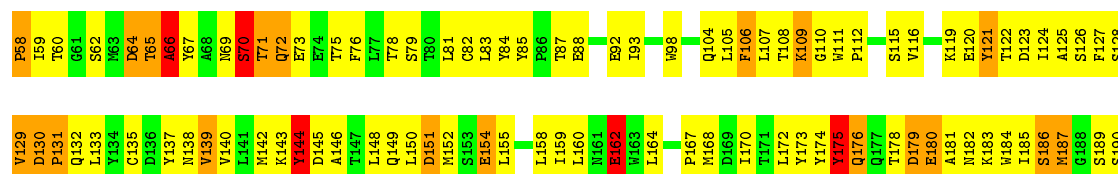


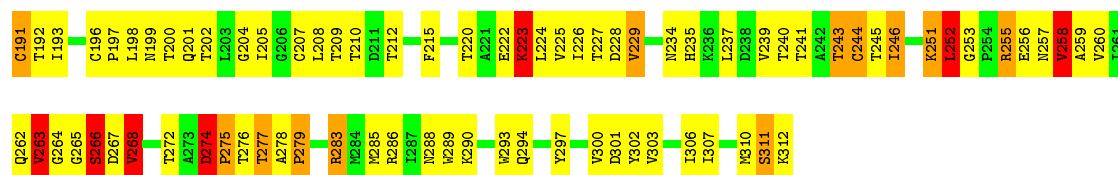
• Molecule 1: Outer capsid glycoprotein VP7



• Molecule 1: Outer capsid glycoprotein VP7

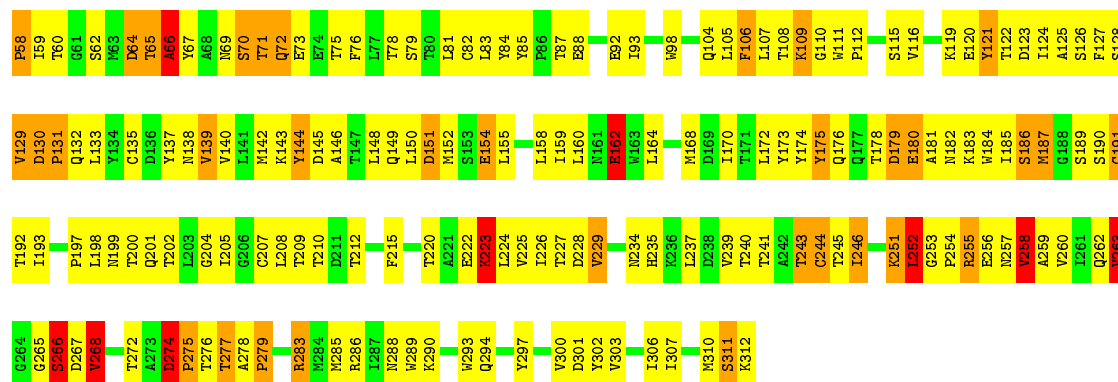






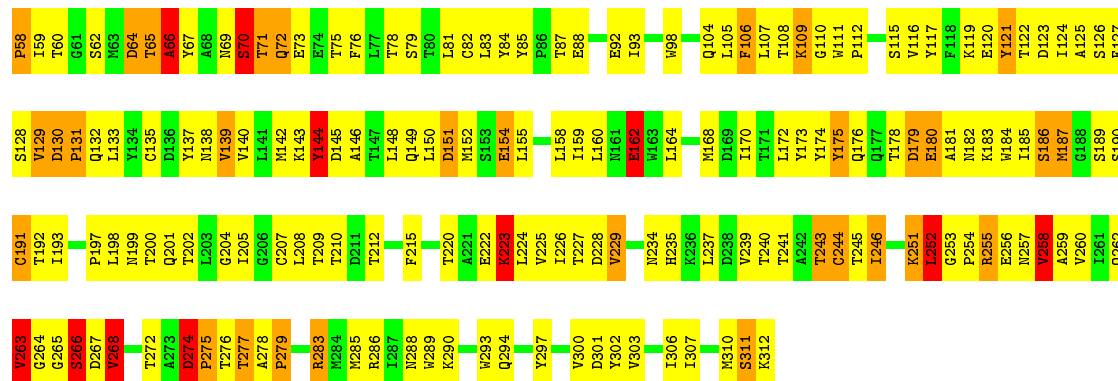
• Molecule 1: Outer capsid glycoprotein VP7

Chain K:



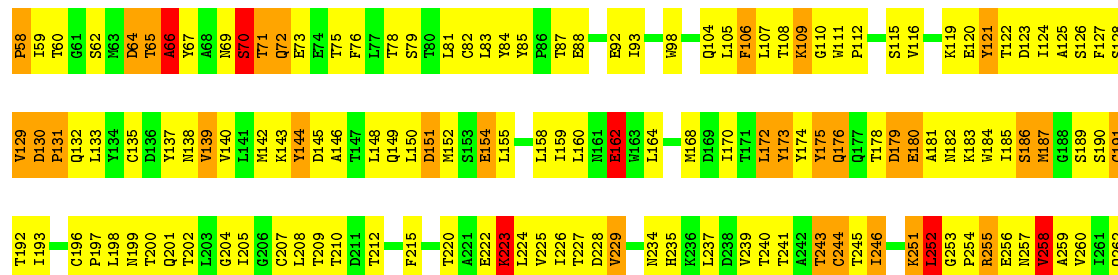
• Molecule 1: Outer capsid glycoprotein VP7

Chain L:



• Molecule 1: Outer capsid glycoprotein VP7

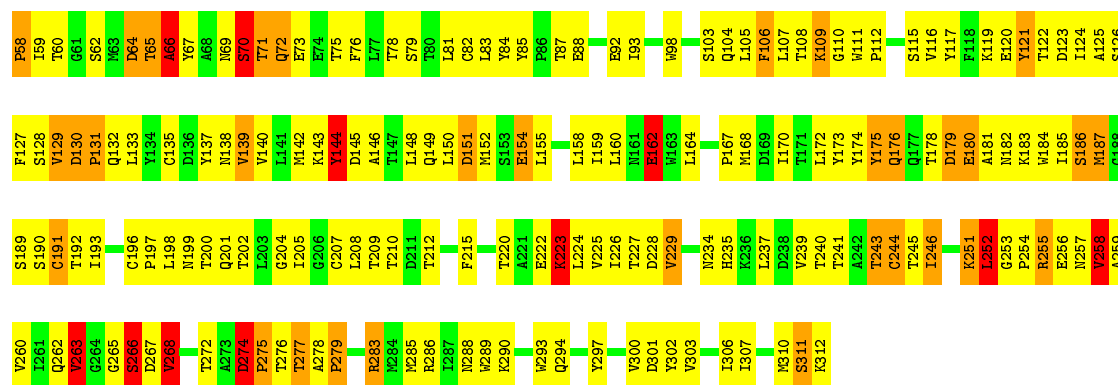
Chain M:





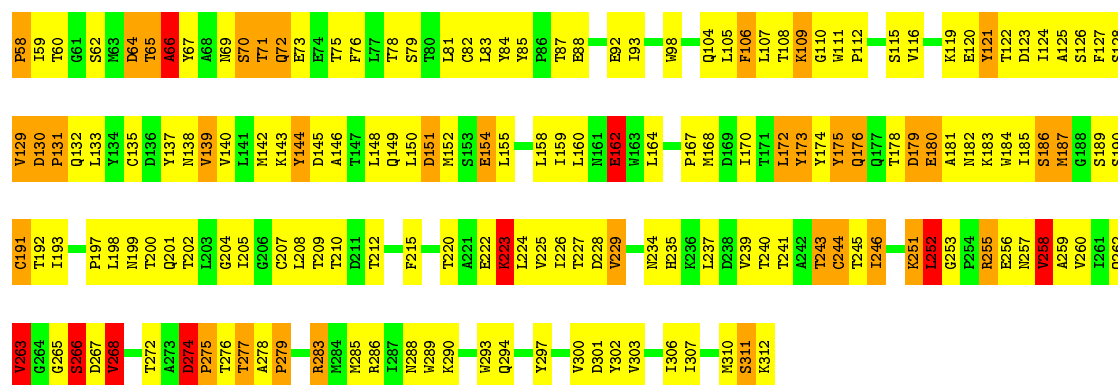
• Molecule 1: Outer capsid glycoprotein VP7

Chain N: 31% 52% 13%



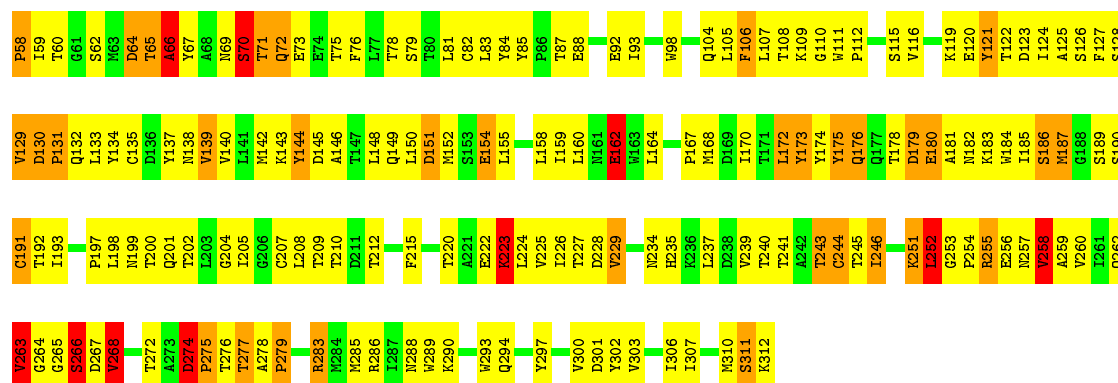
• Molecule 1: Outer capsid glycoprotein VP7

Chain O: 33% 49% 14%

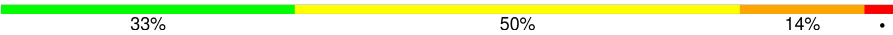


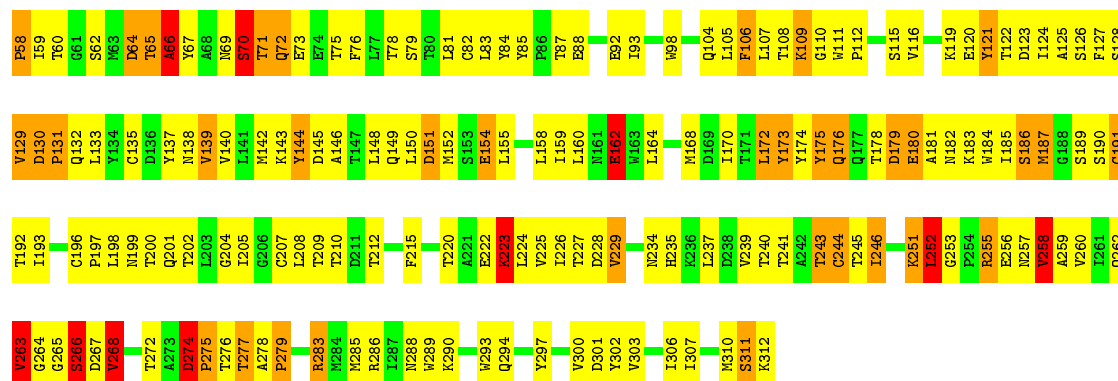
• Molecule 1: Outer capsid glycoprotein VP7

Chain P: 32% 51% 13%



● Molecule 1: Outer capsid glycoprotein VP7

Chain Q:  33% 50% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	individual particle	Depositor
Microscope	TF30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2500	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 > 2$	RMSZ	# $ Z > 2$
1	B	0.81	10/2053 (0.5%)	1.32	32/2806 (1.1%)
1	F	0.82	10/2053 (0.5%)	1.41	39/2806 (1.4%)
1	G	0.95	13/2053 (0.6%)	1.46	38/2806 (1.4%)
1	H	0.87	12/2053 (0.6%)	1.46	39/2806 (1.4%)
1	I	0.88	12/2053 (0.6%)	1.46	37/2806 (1.3%)
1	J	0.87	11/2053 (0.5%)	1.46	41/2806 (1.5%)
1	K	0.87	11/2053 (0.5%)	1.45	37/2806 (1.3%)
1	L	0.87	12/2053 (0.6%)	1.45	39/2806 (1.4%)
1	M	0.87	11/2053 (0.5%)	1.45	38/2806 (1.4%)
1	N	0.87	11/2053 (0.5%)	1.46	38/2806 (1.4%)
1	O	0.87	11/2053 (0.5%)	1.46	37/2806 (1.3%)
1	P	0.87	11/2053 (0.5%)	1.45	38/2806 (1.4%)
1	Q	0.87	11/2053 (0.5%)	1.45	38/2806 (1.4%)
All	All	0.87	146/26689 (0.5%)	1.44	491/36478 (1.3%)

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	3
1	F	0	3
1	G	0	5
1	H	0	4
1	I	0	4
1	J	0	4
1	K	0	4
1	L	0	4
1	M	0	4
1	N	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	4
1	P	0	4
1	Q	0	4
All	All	0	51

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	79	SER	C-N	15.53	1.69	1.34
1	L	66	ALA	C-N	-14.04	1.01	1.34
1	Q	66	ALA	C-N	-14.03	1.01	1.34
1	I	66	ALA	C-N	-14.01	1.01	1.34
1	N	66	ALA	C-N	-14.01	1.01	1.34

The worst 5 of 491 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	66	ALA	O-C-N	-20.72	89.55	122.70
1	N	66	ALA	O-C-N	-20.71	89.57	122.70
1	G	66	ALA	O-C-N	-20.70	89.57	122.70
1	H	66	ALA	O-C-N	-20.70	89.57	122.70
1	P	66	ALA	O-C-N	-20.70	89.57	122.70

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	ASP	Mainchain
1	B	162	GLU	Mainchain
1	B	58	PRO	Mainchain
1	F	130	ASP	Mainchain
1	F	58	PRO	Mainchain

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	B	2011	0	1955	359	0
1	F	2011	0	1952	486	0
1	G	2011	0	1949	494	0
1	H	2011	0	1951	489	0
1	I	2011	0	1951	484	0
1	J	2011	0	1950	487	0
1	K	2011	0	1951	487	0
1	L	2011	0	1950	496	0
1	M	2011	0	1951	488	0
1	N	2011	0	1951	495	0
1	O	2011	0	1951	495	0
1	P	2011	0	1951	498	0
1	Q	2011	0	1951	483	0
2	B	28	0	25	2	0
2	F	28	0	25	2	0
2	G	28	0	25	2	0
2	H	28	0	25	2	0
2	I	28	0	25	2	0
2	J	28	0	25	2	0
2	K	28	0	25	2	0
2	L	28	0	25	2	0
2	M	28	0	25	2	0
2	N	28	0	25	2	0
2	O	28	0	25	2	0
2	P	28	0	25	2	0
2	Q	28	0	25	2	0
3	B	4	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	3	0	0	0	0
3	X	1	0	0	0	0
All	All	26537	0	25689	5475	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 105.

The worst 5 of 5475 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:H:142:MET:HE3	1:H:152:MET:CE	1.33	1.59
1:L:142:MET:CE	1:L:152:MET:HE2	1.31	1.59
1:B:159:ILE:CG2	1:B:258:VAL:HG21	1.14	1.58
1:G:142:MET:CE	1:G:152:MET:HE2	1.31	1.58
1:H:159:ILE:CG2	1:H:258:VAL:HG21	1.14	1.58

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 PDB entries followed by that with respect to all EM entries.

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	B	253/255 (99%)	216 (85%)	26 (10%)	11 (4%)	3	35
1	F	253/255 (99%)	215 (85%)	26 (10%)	12 (5%)	3	33
1	G	253/255 (99%)	215 (85%)	27 (11%)	11 (4%)	3	35
1	H	253/255 (99%)	215 (85%)	26 (10%)	12 (5%)	3	33
1	I	253/255 (99%)	214 (85%)	28 (11%)	11 (4%)	3	35
1	J	253/255 (99%)	216 (85%)	26 (10%)	11 (4%)	3	35
1	K	253/255 (99%)	215 (85%)	27 (11%)	11 (4%)	3	35
1	L	253/255 (99%)	214 (85%)	28 (11%)	11 (4%)	3	35
1	M	253/255 (99%)	215 (85%)	27 (11%)	11 (4%)	3	35
1	N	253/255 (99%)	216 (85%)	26 (10%)	11 (4%)	3	35
1	O	253/255 (99%)	217 (86%)	25 (10%)	11 (4%)	3	35
1	P	253/255 (99%)	216 (85%)	26 (10%)	11 (4%)	3	35
1	Q	253/255 (99%)	215 (85%)	27 (11%)	11 (4%)	3	35
All	All	3289/3315 (99%)	2799 (85%)	345 (10%)	145 (4%)	6	35

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	ASN
1	B	71	THR
1	B	252	LEU
1	B	258	VAL
1	F	252	LEU

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 PDB entries followed by that with respect to all EM entries.

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	B	229/229 (100%)	205 (90%)	24 (10%)	8	41
1	F	229/229 (100%)	205 (90%)	24 (10%)	8	41
1	G	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	H	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	I	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	J	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	K	229/229 (100%)	205 (90%)	24 (10%)	8	41
1	L	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	M	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	N	229/229 (100%)	204 (89%)	25 (11%)	8	40
1	O	229/229 (100%)	205 (90%)	24 (10%)	8	41
1	P	229/229 (100%)	205 (90%)	24 (10%)	8	41
1	Q	229/229 (100%)	204 (89%)	25 (11%)	8	40
All	All	2977/2977 (100%)	2657 (89%)	320 (11%)	13	41

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	268	VAL
1	L	176	GLN
1	Q	70	SER

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Mol	Chain	Res	Type
1	K	106	PHE
1	K	229	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	69	ASN
1	L	235	HIS
1	P	262	GLN
1	K	176	GLN
1	K	257	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 ⓘ

26 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	-	14,14,15	0.59	0	15,19,21	1.19	1 (6%)
2	NAG	B	2	-	14,14,15	1.00	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	F	11	-	14,14,15	0.60	0	15,19,21	1.19	1 (6%)
2	NAG	F	12	-	14,14,15	1.01	1 (7%)	15,19,21	1.72	5 (33%)
2	NAG	G	7	-	14,14,15	0.60	0	15,19,21	1.19	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	8	-	14,14,15	1.01	1 (7%)	15,19,21	1.72	5 (33%)
2	NAG	H	10	-	14,14,15	1.00	1 (7%)	15,19,21	1.72	5 (33%)
2	NAG	H	9	-	14,14,15	0.57	0	15,19,21	1.19	1 (6%)
2	NAG	I	17	-	14,14,15	0.57	0	15,19,21	1.19	1 (6%)
2	NAG	I	18	-	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	J	13	-	14,14,15	0.57	0	15,19,21	1.18	1 (6%)
2	NAG	J	14	-	14,14,15	1.00	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	K	15	-	14,14,15	0.61	0	15,19,21	1.19	1 (6%)
2	NAG	K	16	-	14,14,15	0.99	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	L	23	-	14,14,15	0.58	0	15,19,21	1.20	1 (6%)
2	NAG	L	24	-	14,14,15	1.00	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	M	19	-	14,14,15	0.59	0	15,19,21	1.19	1 (6%)
2	NAG	M	20	-	14,14,15	1.00	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	N	21	-	14,14,15	0.59	0	15,19,21	1.20	1 (6%)
2	NAG	N	22	-	14,14,15	1.00	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	O	29	-	14,14,15	0.59	0	15,19,21	1.19	1 (6%)
2	NAG	O	30	-	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	P	25	-	14,14,15	0.58	0	15,19,21	1.20	1 (6%)
2	NAG	P	26	-	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)
2	NAG	Q	27	-	14,14,15	0.57	0	15,19,21	1.19	1 (6%)
2	NAG	Q	28	-	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)

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	NAG	B	1	-	-	0/6/23/26	0/1/1/1
2	NAG	B	2	-	-	0/6/23/26	0/1/1/1
2	NAG	F	11	-	-	0/6/23/26	0/1/1/1
2	NAG	F	12	-	-	0/6/23/26	0/1/1/1
2	NAG	G	7	-	-	0/6/23/26	0/1/1/1
2	NAG	G	8	-	-	0/6/23/26	0/1/1/1
2	NAG	H	10	-	-	0/6/23/26	0/1/1/1
2	NAG	H	9	-	-	0/6/23/26	0/1/1/1
2	NAG	I	17	-	-	0/6/23/26	0/1/1/1
2	NAG	I	18	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	13	-	-	0/6/23/26	0/1/1/1
2	NAG	J	14	-	-	0/6/23/26	0/1/1/1
2	NAG	K	15	-	-	0/6/23/26	0/1/1/1
2	NAG	K	16	-	-	0/6/23/26	0/1/1/1
2	NAG	L	23	-	-	0/6/23/26	0/1/1/1
2	NAG	L	24	-	-	0/6/23/26	0/1/1/1
2	NAG	M	19	-	-	0/6/23/26	0/1/1/1
2	NAG	M	20	-	-	0/6/23/26	0/1/1/1
2	NAG	N	21	-	-	0/6/23/26	0/1/1/1
2	NAG	N	22	-	-	0/6/23/26	0/1/1/1
2	NAG	O	29	-	-	0/6/23/26	0/1/1/1
2	NAG	O	30	-	-	0/6/23/26	0/1/1/1
2	NAG	P	25	-	-	0/6/23/26	0/1/1/1
2	NAG	P	26	-	-	0/6/23/26	0/1/1/1
2	NAG	Q	27	-	-	0/6/23/26	0/1/1/1
2	NAG	Q	28	-	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	16	NAG	C1-C2	2.73	1.56	1.52
2	L	24	NAG	C1-C2	2.74	1.56	1.52
2	N	22	NAG	C1-C2	2.74	1.56	1.52
2	H	10	NAG	C1-C2	2.75	1.56	1.52
2	J	14	NAG	C1-C2	2.77	1.56	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	16	NAG	O7-C7-C8	-2.62	117.24	122.07
2	N	22	NAG	O7-C7-C8	-2.61	117.26	122.07
2	P	26	NAG	O7-C7-C8	-2.60	117.28	122.07
2	Q	28	NAG	O7-C7-C8	-2.60	117.29	122.07
2	O	30	NAG	O7-C7-C8	-2.60	117.29	122.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	F	11	NAG	2	0
2	G	7	NAG	2	0
2	H	9	NAG	2	0
2	I	17	NAG	2	0
2	J	13	NAG	2	0
2	K	15	NAG	2	0
2	L	23	NAG	2	0
2	M	19	NAG	2	0
2	N	21	NAG	2	0
2	O	29	NAG	2	0
2	P	25	NAG	2	0
2	Q	27	NAG	2	0

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 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.