wwPDB EM Map/Model Validation Report (i)

Apr 26, 2016 – 06:27 PM BST

PDB ID	:	1D3E
EMDB ID:	:	unknown
Title	:	CRYO-EM STRUCTURE OF HUMAN RHINOVIRUS 16 (HRV16) COMPLEXED WITH A TWO-DOMAIN FRAGMENT OF ITS CELLULAR RECEPTOR, INTERCELLULAR ADHESION MOLECULE-1 (D1D2-ICAM-1). IMPLICATIONS FOR VIRUS-RECEPTOR INTERACTIONS. ALPHA CARBONS ONLY
Authors	:	Bella, J.; Rossmann, M.G.
Deposited on	:	1999-09-29
Resolution	:	28.00 Å(reported)

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
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)	:	trunk27461

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 28.00 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	Percentile Ranks	Value
Clashscore		4

Worse *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924

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 <=5%

Mol	Chain	Length	Quality of chain
1	I	185	98% •
2	1	285	100%
3	2	252	99% •
4	3	238	99% •
5	4	68	43% 57%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 989 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 PROTEIN (INTERCELLULAR ADHESION MOLECULE-1).

Mol	Chain	Residues	Atoms		AltConf	Trace
1	I	185	Total C 185 185		0	185

- Molecule 2 is a protein called PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP1).

Mol	Chain	Residues	Atoms		AltConf	Trace
2	1	285	Total C 285 285		0	285

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1	ALA	ASN	CNFLICT	UNP Q82122

- Molecule 3 is a protein called PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP2).

Mol	Chain	Residues	Atoms		AltConf	Trace
3	2	252	Total C 252 252		0	252

- Molecule 4 is a protein called PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP3).

Mol	Chain	Residues	Atoms		AltConf	Trace
4	3	238	Total C 238 238		0	238

- Molecule 5 is a protein called PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP4).

Mol	Chain	Residues	Atoms		AltConf	Trace
5	4	29	Total C 29 29		0	29

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: PROTEIN (INTERCELLULAR ADHESION MOLECULE-1)
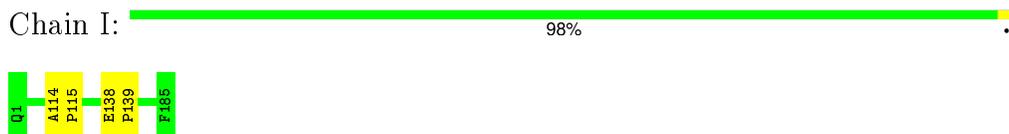
Chain I:

• Molecule 2: PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP1)

Chain 1:

There are no outlier residues recorded for this chain.

• Molecule 3: PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP2)

Chain 2:
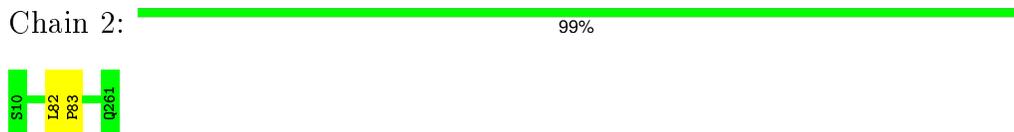
• Molecule 4: PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP3)

Chain 3:
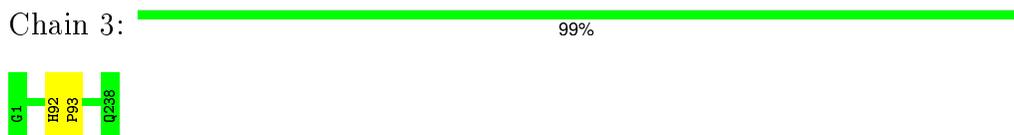
• Molecule 5: PROTEIN (RHINOVIRUS 16 COAT PROTEIN VP4)

Chain 4:
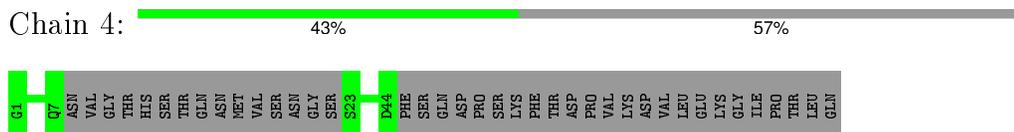
4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	THE RESOLUTION OF THE FINAL RECONSTRUCTED DENSITY WAS DETERMINED TO BE AT LEAST 28 ANGSTROMS, AS MEASURED BY RANDOMLY SPLITTING THE PARTICLES INTO TWO SETS AND COMPARING STRUCTURE FACTORS OBTAINED FROM SEPARATE RECONSTRUCTIONS (BAKER ET AL. 1991, BIOPHYS.J. 60, 1445-1456). THE EIGENVALUE SPECTRUM GAVE AN INDICATION OF THE RANDOMNESS OF THE DATA THAT WAS INCLUDED IN THE RECONSTRUCTION. THE COMPLETENESS OF THE DATA WAS VERIFIED IN THAT ALL EIGENVALUES EXCEEDED 1.0.	Depositor
CTF correction method	Not provided	Depositor
Microscope	PHILLIPS EM240	Depositor
Voltage (kV)	80	Depositor
Electron dose $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	47500	Depositor
Image detector	KODAK SO163 FILM	Depositor

5　Model quality (i)

5.1　Standard geometry (i)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	I	185	0	0	2	0
2	1	285	0	0	0	0
3	2	252	0	0	1	0
4	3	238	0	0	1	0
5	4	29	0	0	0	0
All	All	989	0	0	4	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 4.

All (4) 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:I:138:GLU:CA	1:I:139:PRO:CA	2.89	0.50
1:I:114:ALA:CA	1:I:115:PRO:CA	2.94	0.46
3:2:82:LEU:CA	3:2:83:PRO:CA	2.95	0.45
4:3:92:HIS:CA	4:3:93:PRO:CA	2.98	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

There are no ligands in this entry.

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.