Full wwPDB EM Validation Report (i)

May 14, 2024 – 12:46 am BST

PDB ID	:	6SK6
EMDB ID	:	EMD-10221
Title	:	Cryo-EM structure of rhinovirus-B5
Authors	:	Wald, J.; Goessweiner-Mohr, N.; Blaas, D.; Pasin, M.
Deposited on	:	2019-08-14
Resolution	:	3.20 Å(reported)
Based on initial model	:	1AYM

This is a Full wwPDB EM Validation 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

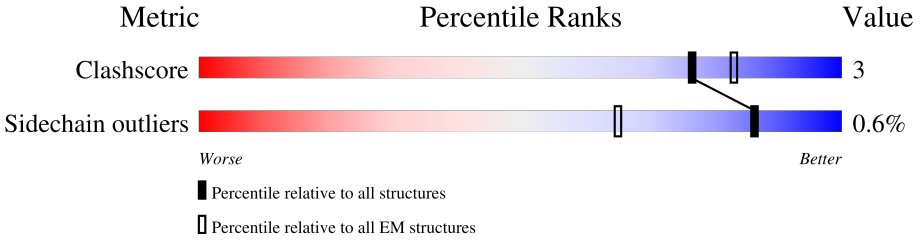
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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	158937	4297
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	D	69	51% 7% 42%
2	B	252	92% 8%
3	A	288	87% 7% • 5%
4	C	231	91% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12352 atoms, of which 6131 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 Rhinovirus B5 VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	D	40	589	188	290	47	62	2	0	0

- Molecule 2 is a protein called Rhinovirus B5 VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	252	3826	1218	1899	320	375	14	0	0

- Molecule 3 is a protein called Rhinovirus B5 VP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	A	273	4340	1383	2147	392	410	8	0	0

- Molecule 4 is a protein called Rhinovirus B5 VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	C	231	3597	1159	1795	294	339	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	THR	ALA	conflict	UNP B9V433

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Rhinovirus B5 VP4

Chain D:

- Molecule 2: Rhinovirus B5 VP2

Chain B:

- Molecule 3: Rhinovirus B5 VP1

Chain A:

- Molecule 4: Rhinovirus B5 VP3

Chain C:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C60	Depositor
Number of particles used	13656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	D	1.05	1/305 (0.3%)	0.67	0/409
2	B	1.31	9/1971 (0.5%)	0.64	0/2684
3	A	1.35	13/2252 (0.6%)	0.68	0/3063
4	C	1.33	7/1850 (0.4%)	0.70	1/2530 (0.0%)
All	All	1.32	30/6378 (0.5%)	0.67	1/8686 (0.0%)

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
3	A	0	3
4	C	0	2
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	38	GLU	CG-CD	-7.54	1.40	1.51
3	A	204	TYR	CB-CG	-7.29	1.40	1.51
3	A	259	ARG	CG-CD	-6.90	1.34	1.51
3	A	190	TYR	CB-CG	-6.88	1.41	1.51
4	C	112	ARG	CB-CG	-6.34	1.35	1.52
4	C	117	TYR	CE2-CZ	-6.14	1.30	1.38
4	C	186	PHE	CB-CG	-6.02	1.41	1.51
4	C	112	ARG	CG-CD	-5.98	1.37	1.51
3	A	128	TYR	CB-CG	-5.86	1.42	1.51
2	B	32	ILE	CB-CG1	-5.84	1.37	1.54
3	A	124	PHE	CG-CD2	-5.78	1.30	1.38
2	B	125	VAL	CB-CG2	-5.67	1.41	1.52
3	A	244	TYR	CB-CG	-5.67	1.43	1.51
3	A	77	VAL	CB-CG2	-5.67	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	TRP	CB-CG	-5.66	1.40	1.50
2	B	247	PHE	CG-CD1	-5.66	1.30	1.38
3	A	122	VAL	CB-CG1	-5.62	1.41	1.52
1	D	57	VAL	CB-CG1	-5.61	1.41	1.52
2	B	112	CYS	CB-SG	-5.54	1.72	1.81
3	A	38	GLU	CD-OE1	-5.51	1.19	1.25
4	C	28	TYR	CB-CG	-5.50	1.43	1.51
3	A	263	TYR	CB-CG	-5.50	1.43	1.51
2	B	106	TYR	CB-CG	-5.38	1.43	1.51
4	C	28	TYR	CG-CD2	-5.26	1.32	1.39
2	B	183	PHE	CB-CG	-5.18	1.42	1.51
2	B	170	TYR	CB-CG	-5.14	1.44	1.51
2	B	121	CYS	CB-SG	-5.14	1.73	1.81
4	C	39	GLU	CD-OE1	-5.13	1.20	1.25
3	A	38	GLU	CD-OE2	-5.08	1.20	1.25
3	A	176	VAL	CB-CG1	-5.02	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	142	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	109	LEU	Mainchain,Peptide
3	A	99	PHE	Mainchain
4	C	72	VAL	Mainchain,Peptide

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	D	299	290	290	2	0
2	B	1927	1899	1899	9	0
3	A	2193	2147	2147	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1802	1795	1795	18	0
All	All	6221	6131	6131	37	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 3.

All (37) 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:B:254:ARG:NH2	2:B:257:ALA:HB2	2.00	0.77
4:C:42:ASN:ND2	4:C:44:LEU:HB2	2.06	0.70
3:A:42:THR:HG22	3:A:42:THR:O	1.92	0.68
4:C:42:ASN:HD21	4:C:44:LEU:HD12	1.59	0.67
3:A:38:GLU:OE1	3:A:38:GLU:N	2.31	0.61
3:A:99:PHE:O	3:A:99:PHE:CG	2.52	0.60
2:B:227:ILE:HG23	2:B:227:ILE:O	2.02	0.58
3:A:65:THR:HG1	4:C:42:ASN:CG	2.05	0.57
3:A:65:THR:OG1	4:C:42:ASN:OD1	2.10	0.56
4:C:87:LEU:HD22	4:C:107:TRP:CG	2.41	0.56
2:B:76:LYS:HD2	2:B:156:LEU:O	2.09	0.52
4:C:161:VAL:O	4:C:161:VAL:HG13	2.09	0.51
3:A:45:THR:HG22	3:A:46:THR:N	2.27	0.48
2:B:254:ARG:HH21	2:B:257:ALA:HB2	1.74	0.48
3:A:65:THR:O	4:C:42:ASN:OD1	2.32	0.48
4:C:87:LEU:HD22	4:C:107:TRP:CD2	2.51	0.46
3:A:65:THR:C	4:C:42:ASN:OD1	2.54	0.46
3:A:138:ASN:OD1	3:A:138:ASN:C	2.55	0.45
2:B:158:GLU:O	2:B:166:LYS:NZ	2.49	0.45
2:B:227:ILE:O	2:B:227:ILE:CG2	2.65	0.45
3:A:204:TYR:CD1	3:A:204:TYR:N	2.86	0.44
3:A:282:ARG:NH1	3:A:287:THR:O	2.51	0.43
2:B:191:ARG:NH1	4:C:120:PRO:O	2.52	0.43
2:B:204:ASN:OD1	2:B:205:SER:N	2.52	0.43
3:A:254:VAL:HG12	3:A:254:VAL:O	2.19	0.43
4:C:42:ASN:HD22	4:C:44:LEU:HB2	1.83	0.43
1:D:55:GLU:N	1:D:56:PRO:CD	2.82	0.42
3:A:99:PHE:O	3:A:99:PHE:CD2	2.72	0.42
4:C:87:LEU:CD2	4:C:107:TRP:CG	3.03	0.42
4:C:42:ASN:ND2	4:C:44:LEU:HD12	2.31	0.42
4:C:198:PRO:HA	4:C:199:PRO:HD3	1.90	0.42
2:B:16:ILE:N	2:B:16:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:107:TRP:CH2	4:C:167:TRP:HZ3	2.39	0.41
4:C:155:ILE:O	4:C:155:ILE:HG22	2.21	0.41
4:C:193:THR:OG1	4:C:194:SER:N	2.53	0.41
1:D:49:ASP:OD2	1:D:52:LYS:NZ	2.51	0.40
4:C:21:SER:HA	4:C:22:PRO:HD3	1.94	0.40

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)

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	D	33/58 (57%)	33 (100%)	0	100	100
2	B	219/219 (100%)	217 (99%)	2 (1%)	78	91
3	A	245/258 (95%)	243 (99%)	2 (1%)	81	93
4	C	202/202 (100%)	202 (100%)	0	100	100
All	All	699/737 (95%)	695 (99%)	4 (1%)	86	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	226	ASP
2	B	254	ARG
3	A	99	PHE
3	A	220	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 monosaccharides 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.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10221. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.