



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:07 am GMT

PDB ID : 1Z7Z
EMDB ID: : EMD-1114
Title : Cryo-em structure of human coxsackievirus A21 complexed with five domain icam-1kilifi
Authors : Xiao, C.; Bator-Kelly, C.M.; Rieder, E.; Chipman, P.R.; Craig, A.; Kuhn, R.J.; Wimmer, E.; Rossmann, M.G.
Deposited on : 2005-03-28
Resolution : 8.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

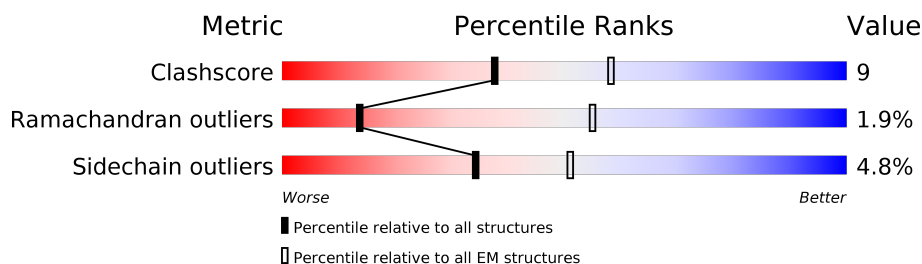
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1	286	67% 6% • 25%
2	2	272	87% 8% • •
3	3	234	74% 8% 18%
4	4	12	92% 8%
5	5	6	50% 17% 17% 17%
6	I	450	74% 20% • •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8824 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 human coxsackievirus A21.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	214	Total	C	N	O	S	0	0
			1723	1102	295	317	9		

- Molecule 2 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	263	Total	C	N	O	S	0	0
			2042	1297	345	389	11		

- Molecule 3 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	192	Total	C	N	O	S	0	0
			1493	955	246	274	18		

- Molecule 4 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	12	Total	C	N	O	0	0
			94	62	13	19		

- Molecule 5 is a protein called human coxsackievirus A21.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	5	Total	C	N	O	0	0
			38	24	8	6		

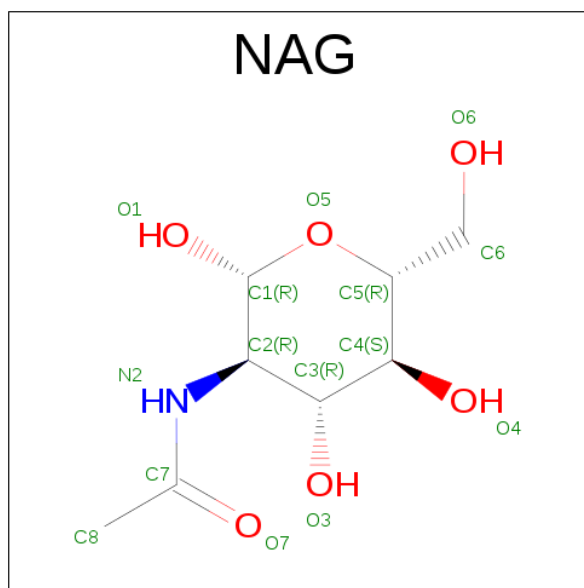
- Molecule 6 is a protein called Intercellular adhesion molecule-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	434	Total	C	N	O	S	0	0
			3322	2073	577	655	17		

There is a discrepancy between the modelled and reference sequences:

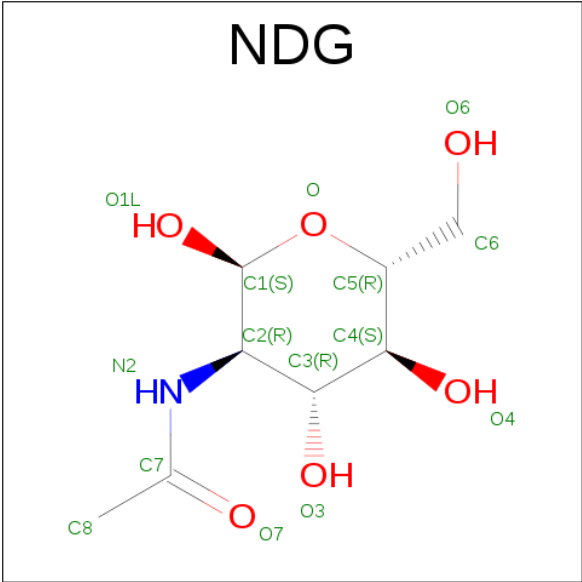
Chain	Residue	Modelled	Actual	Comment	Reference
I	29	MET	LYS	ENGINEERED	UNP P05362

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	I	1	Total	C	N	O	0
			98	56	7	35	
7	I	1	Total	C	N	O	0
			98	56	7	35	
7	I	1	Total	C	N	O	0
			98	56	7	35	
7	I	1	Total	C	N	O	0
			98	56	7	35	
7	I	1	Total	C	N	O	0
			98	56	7	35	
7	I	1	Total	C	N	O	0
			98	56	7	35	

- Molecule 8 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).

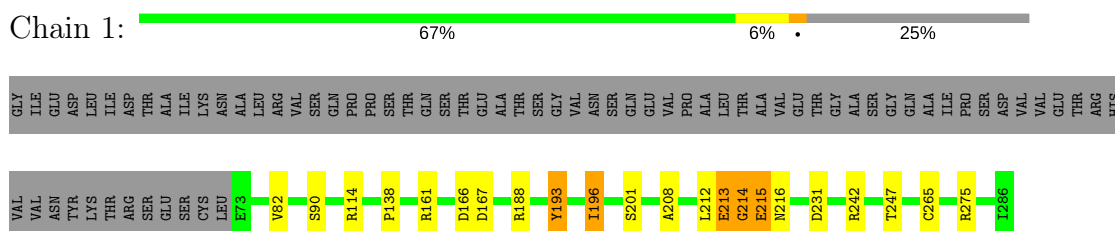


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	I	1	14	8	1	5	0

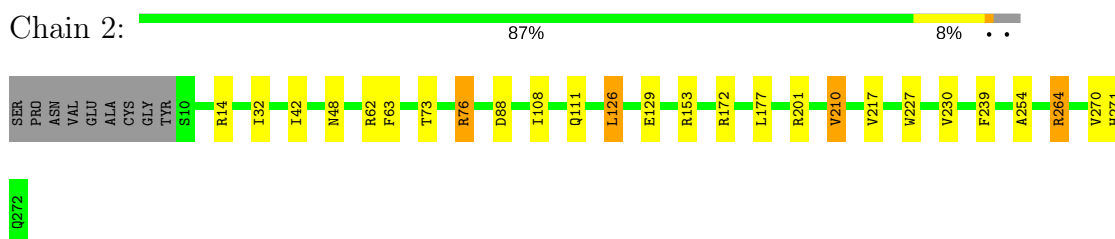
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

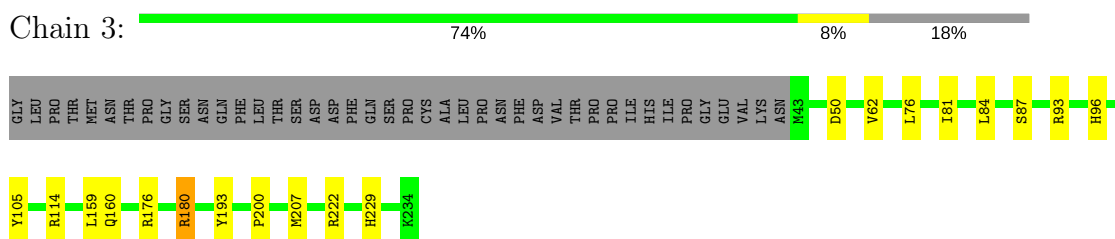
- Molecule 1: human coxsackievirus A21



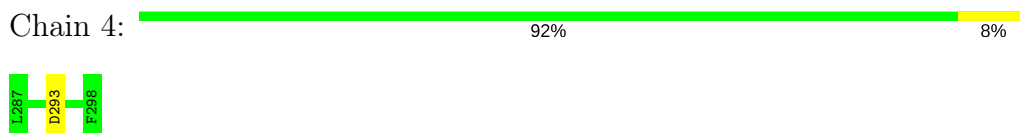
- Molecule 2: human coxsackievirus A21



- Molecule 3: human coxsackievirus A21

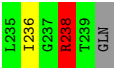


- Molecule 4: human coxsackievirus A21



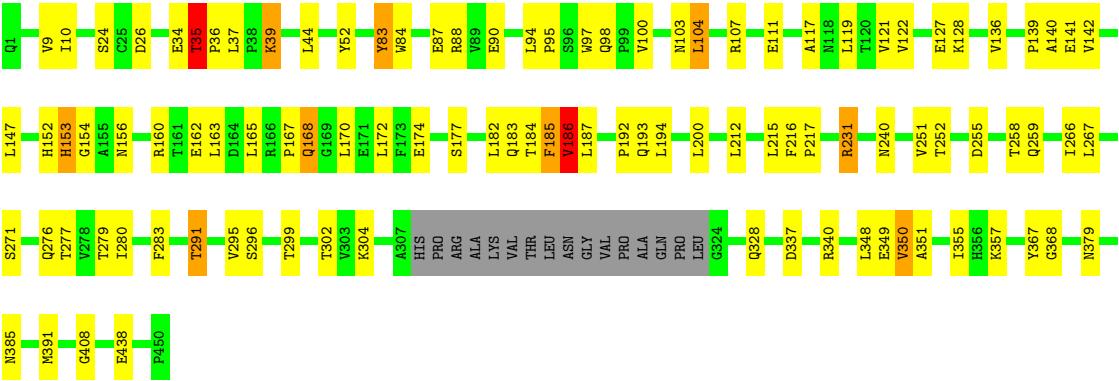
- Molecule 5: human coxsackievirus A21





● Molecule 6: Intercellular adhesion molecule-1

Chain I: 74% 20% ● ●



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	REVERSED CTF WITH WEINER FACTOR FOR EACH PARTICLE	Depositor
Microscope	FEG300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2600	Depositor
Minimum defocus (nm)	700.00	Depositor
Maximum defocus (nm)	3000.00	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO163 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: NAG, NDG

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	1	0.77	0/1777	1.06	3/2419 (0.1%)
2	2	0.71	0/2098	1.03	6/2870 (0.2%)
3	3	0.71	0/1531	1.06	4/2078 (0.2%)
4	4	0.70	0/95	1.02	0/128
5	5	0.74	0/37	1.95	1/48 (2.1%)
6	I	0.50	0/3388	0.83	3/4629 (0.1%)
All	All	0.65	0/8926	0.98	17/12172 (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	1	0	1
2	2	0	1
3	3	0	3
5	5	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	76	ARG	NE-CZ-NH2	-8.53	116.04	120.30
6	I	186	VAL	CA-C-N	-7.40	100.92	117.20
5	5	238	ARG	NE-CZ-NH1	7.15	123.88	120.30
2	2	264	ARG	NE-CZ-NH1	7.04	123.82	120.30
3	3	114	ARG	NE-CZ-NH1	6.64	123.62	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	TYR	Sidechain
2	2	172	ARG	Sidechain
3	3	105	TYR	Sidechain
3	3	87	SER	Peptide
3	3	93	ARG	Sidechain

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	1	1723	0	1648	17	0
2	2	2042	0	1966	12	0
3	3	1493	0	1490	3	0
4	4	94	0	100	0	0
5	5	38	0	44	0	0
6	I	3322	0	3303	124	0
7	I	98	0	91	11	0
8	I	14	0	13	6	0
All	All	8824	0	8655	149	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 9.

The worst 5 of 149 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)
6:I:103:ASN:HD21	7:I:451:NAG:C1	0.93	1.58
6:I:279:THR:CG2	6:I:350:VAL:HG23	1.23	1.55
6:I:279:THR:CG2	6:I:350:VAL:CG2	2.02	1.38
6:I:279:THR:HG21	6:I:350:VAL:CG2	1.52	1.37
6:I:279:THR:CB	6:I:350:VAL:HG23	1.55	1.34

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	1	212/286 (74%)	185 (87%)	19 (9%)	8 (4%)	4	32
2	2	261/272 (96%)	242 (93%)	17 (6%)	2 (1%)	22	67
3	3	190/234 (81%)	176 (93%)	13 (7%)	1 (0%)	32	74
4	4	10/12 (83%)	10 (100%)	0	0	100	100
5	5	3/6 (50%)	1 (33%)	0	2 (67%)	0	0
6	I	430/450 (96%)	407 (95%)	15 (4%)	8 (2%)	9	47
All	All	1106/1260 (88%)	1021 (92%)	64 (6%)	21 (2%)	14	47

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	213	GLU
1	1	214	GLY
5	5	238	ARG
6	I	35	THR
6	I	36	PRO

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	1	188/249 (76%)	182 (97%)	6 (3%)	44	71
2	2	223/230 (97%)	212 (95%)	11 (5%)	29	61
3	3	170/208 (82%)	163 (96%)	7 (4%)	35	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	12/12 (100%)	11 (92%)	1 (8%)	13	43
5	5	4/5 (80%)	4 (100%)	0	100	100
6	I	382/395 (97%)	360 (94%)	22 (6%)	23	56
All	All	979/1099 (89%)	932 (95%)	47 (5%)	34	61

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	160	GLN
6	I	24	SER
6	I	379	ASN
3	3	207	MET
6	I	35	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
6	I	103	ASN
6	I	153	HIS
6	I	388	GLN
6	I	98	GLN
6	I	379	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands 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$
7	NAG	I	451	6	14,14,15	3.65	2 (14%)	15,19,21	2.09	3 (20%)
7	NAG	I	452	6	14,14,15	0.66	0	15,19,21	1.30	2 (13%)
7	NAG	I	453	6	14,14,15	0.70	0	15,19,21	0.90	0
7	NAG	I	454	6	14,14,15	0.57	0	15,19,21	0.79	1 (6%)
7	NAG	I	455	-	14,14,15	0.70	0	15,19,21	1.12	1 (6%)
7	NAG	I	456	6	14,14,15	0.76	0	15,19,21	1.36	4 (26%)
8	NDG	I	457	6	14,14,15	0.71	1 (7%)	15,19,21	0.76	0
7	NAG	I	458	6	14,14,15	0.61	0	15,19,21	0.70	0

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
7	NAG	I	451	6	-	0/6/23/26	0/1/1/1
7	NAG	I	452	6	-	0/6/23/26	0/1/1/1
7	NAG	I	453	6	-	0/6/23/26	0/1/1/1
7	NAG	I	454	6	-	0/6/23/26	0/1/1/1
7	NAG	I	455	-	-	0/6/23/26	0/1/1/1
7	NAG	I	456	6	-	0/6/23/26	0/1/1/1
8	NDG	I	457	6	-	1/6/23/26	0/1/1/1
7	NAG	I	458	6	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	457	NDG	C1-C2	2.07	1.55	1.52
7	I	451	NAG	C3-C2	4.57	1.62	1.52
7	I	451	NAG	C1-C2	12.42	1.69	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	455	NAG	C2-N2-C7	-3.05	118.49	122.94
7	I	456	NAG	O5-C1-C2	-2.75	107.65	111.47
7	I	452	NAG	C3-C4-C5	-2.69	105.48	110.22
7	I	451	NAG	O7-C7-C8	-2.19	118.07	122.06
7	I	454	NAG	C2-N2-C7	-2.08	119.91	122.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	458	NAG	O7-C7-N2-C2
8	I	457	NDG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	451	NAG	4	0
7	I	452	NAG	4	0
7	I	454	NAG	1	0
7	I	455	NAG	2	0
7	I	456	NAG	1	0
8	I	457	NDG	6	0

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.