



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4JGZ
Title : Crystal structure of human coxsackievirus A16 uncoating intermediate (space group I222)
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Deposited on : 2013-03-04
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

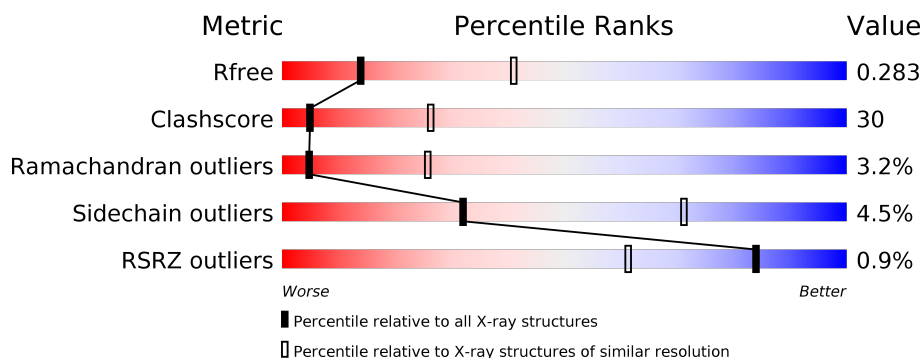
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 on the lower 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 $\leq 5\%$. 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	297	<div> <div> <div></div> <div>35%</div> <div>39%</div> <div>23%</div> </div> <div> <div></div> <div>35%</div> <div>39%</div> <div>23%</div> </div> </div>
2	B	254	<div> <div> <div></div> <div>46%</div> <div>45%</div> <div>6%</div> </div> <div> <div></div> <div>46%</div> <div>45%</div> <div>6%</div> </div> </div>
3	C	242	<div> <div> <div></div> <div>48%</div> <div>44%</div> <div>5%</div> </div> <div> <div></div> <div>48%</div> <div>44%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5468 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 Polyprotein, capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1830	1170	312	335	13			

- Molecule 2 is a protein called Polyprotein, capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1844	1186	305	343	10			

- Molecule 3 is a protein called Polyprotein, capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	231	Total	C	N	O	S	0	0	0
			1794	1156	291	336	11			

- Molecule 1: Polyprotein, capsid protein VP1



G1	K78	Q162	P234
K7	T79	Q167	I235
G9	E81	L168	E236
T10	L82	V169	GLN
N11	G83	P170	THR
Q12	A84	W171	ASN
F13	R87	I172	ILE
L14	A88	S173	GLN
T15	D89	NH74	
T16	P90	T175	
D17	G91	H176	
D18	R92	Y177	
G19	D93	R178	
V20	G94	A179	
S21	Q97	HIS	
I24	S98	ALA	
L25	T99	ARG	
T31	I100	ALA	
I34	C105	GLY	
P37	R106	Y185	
G38	Y107	F186	
E39	Y108	Y189	
V40	T109	I193	
H41	Q110	I194	
M42	W111	T195	
L43	S112	I196	
L44	G113	W197	
E45	S114	Y198	
R48	L115	N201	
V49	F121	Y202	
E50	A122	V203	
T51	G123	V204	
E54	S124	P205	
V55	F125	I206	
N56	M126	G207	
N57	M131	A208	
L58	L132	I214	
N61	I133	L217	
P65	T136	A218	
M66	P143	A219	
Q67	A144	A220	
R68	D145	Q221	
F71	R146	D222	
P72	I147	N223	
V73	T148	F224	
S74	A149	T225	
V75	A149	N226	
Q76	H154	K227	
S77	V155	L228	
	I156	C229	
	F159	T232	
		E233	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	338.40Å 360.20Å 366.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 3.00 49.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	24.5 (49.46-3.00) 24.5 (49.46-3.00)	Depositor EDS
R_{merge}	0.46	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.01Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.286 , 0.311 0.288 , 0.283	Depositor DCC
R_{free} test set	5344 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.147 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

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	0.39	0/1883	0.64	0/2564
2	B	0.38	0/1898	0.65	0/2608
3	C	0.40	0/1845	0.67	0/2528
All	All	0.39	0/5626	0.65	0/7700

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

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	1830	0	1792	127	0
2	B	1844	0	1786	127	0
3	C	1794	0	1759	121	0
All	All	5468	0	5337	326	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 30.

The worst 5 of 326 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:181:GLN:HG2	2:B:191:ALA:HB1	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLN:HG2	3:C:21:SER:HB3	1.45	0.98
2:B:134:THR:HG22	2:B:135:ILE:H	1.32	0.93
1:A:139:VAL:HG12	1:A:249:LEU:HB2	1.49	0.91
3:C:65:PRO:O	3:C:68:ARG:HG3	1.75	0.87

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	224/297 (75%)	193 (86%)	22 (10%)	9 (4%)	3	20
2	B	235/254 (92%)	191 (81%)	36 (15%)	8 (3%)	4	24
3	C	227/242 (94%)	196 (86%)	26 (12%)	5 (2%)	8	36
All	All	686/793 (86%)	580 (84%)	84 (12%)	22 (3%)	5	26

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	PRO
2	B	58	VAL
2	B	144	SER
1	A	124	GLU
2	B	29	ALA

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 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	204/257 (79%)	196 (96%)	8 (4%)	37	75
2	B	202/212 (95%)	195 (96%)	7 (4%)	41	78
3	C	197/204 (97%)	185 (94%)	12 (6%)	22	59
All	All	603/673 (90%)	576 (96%)	27 (4%)	32	71

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	155	GLN
3	C	13	PHE
3	C	225	THR
2	B	190	CYS
1	A	235	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	15	GLN
2	B	94	GLN
2	B	225	ASN
1	A	278	ASN
3	C	11	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 [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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	228/297 (76%)	-0.50	2 (0%) 84 61	14, 48, 125, 173	0
2	B	239/254 (94%)	-0.34	4 (1%) 70 42	23, 52, 157, 194	0
3	C	231/242 (95%)	-0.59	0 100 100	16, 42, 105, 139	0
All	All	698/793 (88%)	-0.48	6 (0%) 84 61	14, 46, 140, 194	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	50	VAL	2.9
1	A	100	THR	2.7
2	B	11	ASP	2.6
2	B	143	ASN	2.5
1	A	73	HIS	2.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.