wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2023 – 12:18 AM EST

PDB ID	:	1AYN
Title	:	HUMAN RHINOVIRUS 16 COAT PROTEIN
Authors	:	Hadfield, A.T.; Oliveira, M.A.; Zhao, R.; Rossmann, M.G.
Deposited on	:	1997-11-06
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
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 (1)) were used in the production of this report:

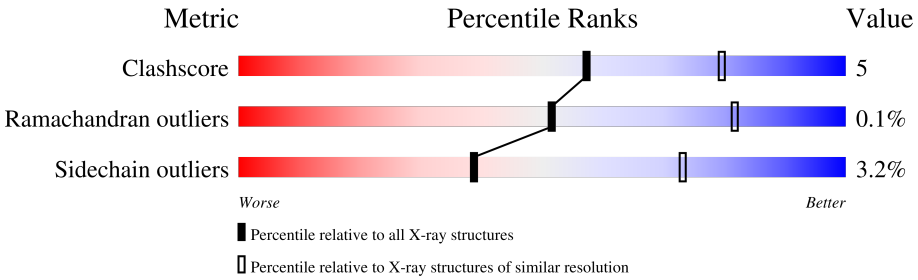
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 of the lower 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	1	285	80% 19% .
2	2	261	87% 10% .
3	3	238	92% 7% .
4	4	68	28% 13% . 57%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6674 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 HUMAN RHINOVIRUS 16 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	285	Total	C	N	O	S	0	0	0
			2287	1442	397	437	11			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 16 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	252	Total	C	N	O	S	0	0	0
			1977	1252	343	372	10			

- Molecule 3 is a protein called HUMAN RHINOVIRUS 16 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1845	1186	298	346	15			

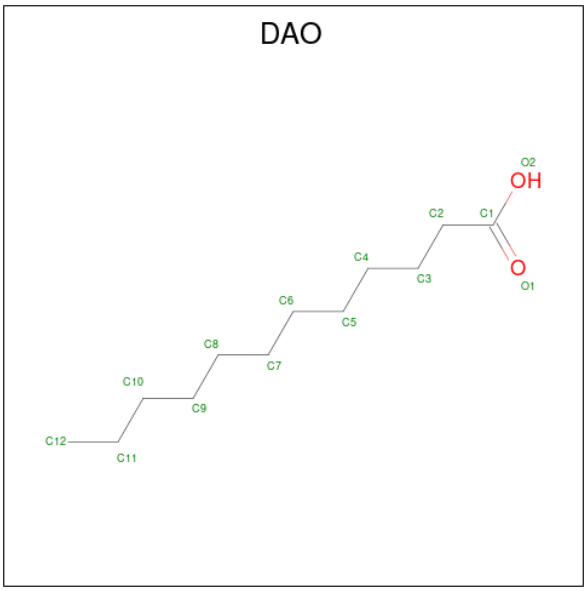
- Molecule 4 is a protein called HUMAN RHINOVIRUS 16 COAT PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	29	Total	C	N	O	0	0	0
			224	138	41	45			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

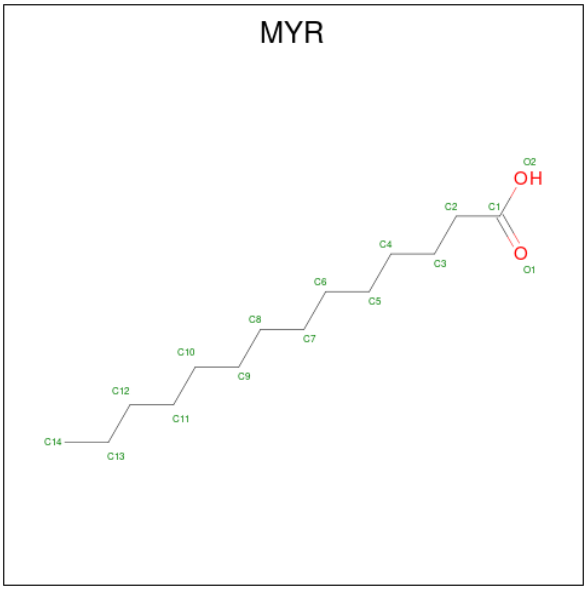
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	1	Total	Zn	0	0
			1	1		

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	1	Total C O 14 12 2	0	0

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	4	1	Total C O 15 14 1	0	0

- Molecule 8 is water.

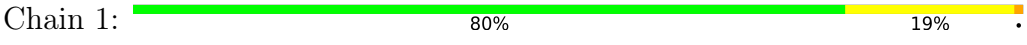
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	1	103	Total O 103 103	0	0
8	2	113	Total O 113 113	0	0
8	3	91	Total O 91 91	0	0
8	4	4	Total O 4 4	0	0

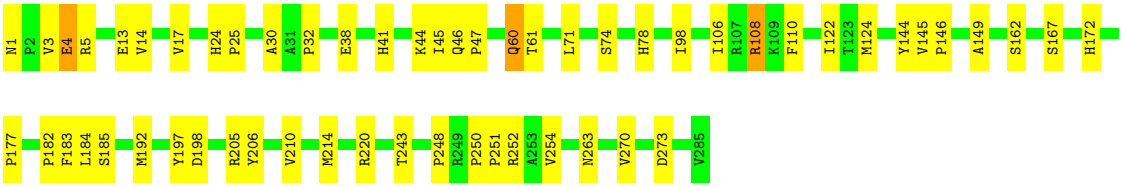
3 Residue-property plots (i)

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: HUMAN RHINOVIRUS 16 COAT PROTEIN

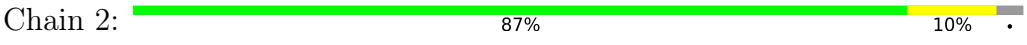
Chain 1:

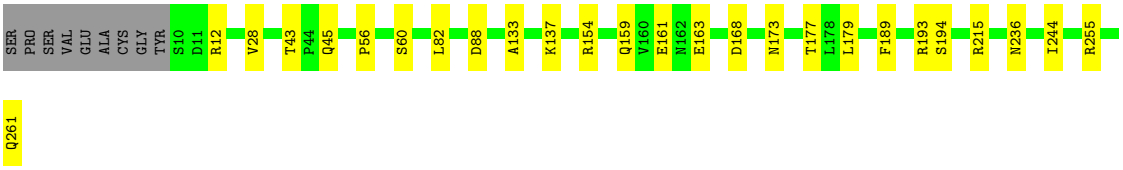




• Molecule 2: HUMAN RHINOVIRUS 16 COAT PROTEIN

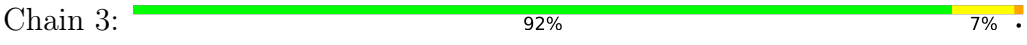
Chain 2:





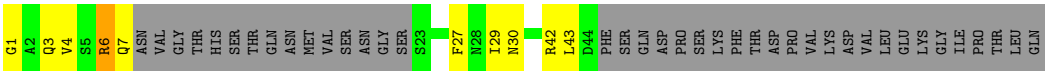
• Molecule 3: HUMAN RHINOVIRUS 16 COAT PROTEIN

Chain 3:



• Molecule 4: HUMAN RHINOVIRUS 16 COAT PROTEIN

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	362.60Å 347.10Å 334.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90 29.95 – 2.85	Depositor EDS
% Data completeness (in resolution range)	63.1 (8.00-2.90) 49.5 (29.95-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.70 (at 2.85Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.229 , 0.230 0.088 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6674	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, ZN, DAO

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	1	0.39	0/2349	0.65	1/3204 (0.0%)
2	2	0.43	0/2029	0.69	0/2770
3	3	0.40	0/1897	0.66	0/2596
4	4	0.56	0/226	1.06	2/301 (0.7%)
All	All	0.41	0/6501	0.68	3/8871 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	220	ARG	NE-CZ-NH2	7.10	123.85	120.30
4	4	6	ARG	NE-CZ-NH2	7.09	123.84	120.30
4	4	42	ARG	NE-CZ-NH2	6.41	123.50	120.30

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	1	2287	0	2201	37	0
2	2	1977	0	1920	16	0
3	3	1845	0	1826	11	0
4	4	224	0	208	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1	1	0	0	0	0
6	1	14	0	23	4	0
7	4	15	0	27	0	0
8	1	103	0	0	2	0
8	2	113	0	0	0	0
8	3	91	0	0	1	0
8	4	4	0	0	0	0
All	All	6674	0	6205	62	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 5.

The worst 5 of 62 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)
2:2:154:ARG:NH1	2:2:159:GLN:HG2	1.93	0.82
1:1:13:GLU:HA	1:1:61:THR:HG21	1.61	0.82
2:2:154:ARG:HH12	2:2:159:GLN:HG2	1.49	0.75
2:2:56:PRO:HB2	2:2:60:SER:HB2	1.73	0.70
2:2:173:ASN:HD21	2:2:179:LEU:HA	1.58	0.67

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	1	283/285 (99%)	272 (96%)	11 (4%)	0	100 100
2	2	250/261 (96%)	232 (93%)	17 (7%)	1 (0%)	34 66
3	3	236/238 (99%)	225 (95%)	11 (5%)	0	100 100
4	4	25/68 (37%)	24 (96%)	1 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	794/852 (93%)	753 (95%)	40 (5%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	161	GLU

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	1	256/256 (100%)	247 (96%)	9 (4%)	36 70
2	2	221/228 (97%)	215 (97%)	6 (3%)	44 77
3	3	210/210 (100%)	205 (98%)	5 (2%)	49 79
4	4	23/59 (39%)	20 (87%)	3 (13%)	4 12
All	All	710/753 (94%)	687 (97%)	23 (3%)	39 73

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	261	GLN
3	3	178	THR
3	3	159	LEU
3	3	182	THR
1	1	162	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	108	HIS
3	3	61	ASN
2	2	232	ASN
2	2	173	ASN

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Mol	Chain	Res	Type
3	3	59	GLN

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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	MYR	4	4000	4	14,14,15	0.41	0	13,13,15	0.61	0
6	DAO	1	7009	-	13,13,13	0.97	1 (7%)	13,13,13	0.79	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	MYR	4	4000	4	-	6/11/12/13	-
6	DAO	1	7009	-	-	7/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	7009	DAO	C2-C1	2.46	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	7009	DAO	C1-C2-C3-C4
7	4	4000	MYR	C4-C5-C6-C7
7	4	4000	MYR	C6-C7-C8-C9
6	1	7009	DAO	C6-C7-C8-C9
6	1	7009	DAO	C5-C6-C7-C8

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	7009	DAO	4	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.