wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 11:02 PM EST

PDB ID	:	2OQ0
Title	:	Crystal Structure of the First HIN-200 Domain of Interferon-Inducible Protein 16
Authors	:	Lam, R.; Liao, J.C.C.; Ravichandran, M.; Ma, J.; Tempel, W.; Chirgadze, N.Y.; Arrowsmith, C.H.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2007-01-30
Resolution	:	2.00 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
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 (i)) were used in the production of this report:

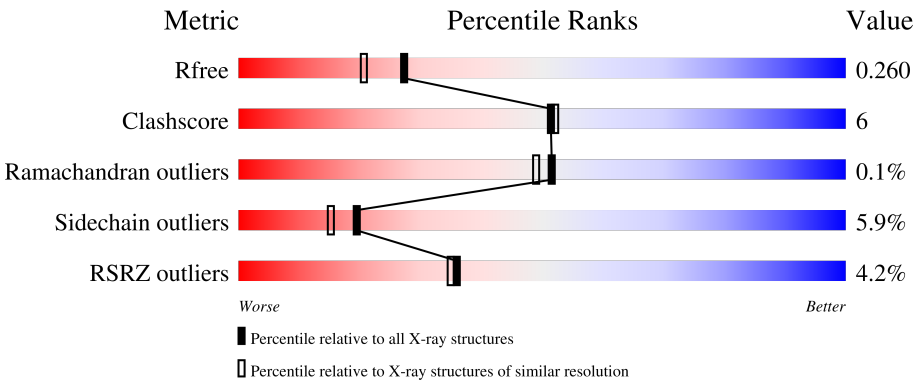
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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% 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	206	3% 77% 14% • 8%
1	B	206	% 72% 19% • 7%
1	C	206	2% 77% 16% • 7%
1	D	206	9% 75% 14% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6320 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 Gamma-interferon-inducible protein Ifi-16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	189	1544	988	264	284	3	5	0	2	0
1	B	192	1561	1000	264	288	3	6	0	1	0
1	C	192	1555	993	264	289	3	6	0	0	0
1	D	184	1500	962	254	275	3	6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q16666
A	2	SER	-	cloning artifact	UNP Q16666
A	3	HIS	-	cloning artifact	UNP Q16666
A	4	MSE	-	cloning artifact	UNP Q16666
A	36	MSE	MET	modified residue	UNP Q16666
A	41	MSE	MET	modified residue	UNP Q16666
A	134	MSE	MET	modified residue	UNP Q16666
A	156	MSE	MET	modified residue	UNP Q16666
A	188	MSE	MET	modified residue	UNP Q16666
A	195	MSE	MET	modified residue	UNP Q16666
B	1	GLY	-	cloning artifact	UNP Q16666
B	2	SER	-	cloning artifact	UNP Q16666
B	3	HIS	-	cloning artifact	UNP Q16666
B	4	MSE	-	cloning artifact	UNP Q16666
B	36	MSE	MET	modified residue	UNP Q16666
B	41	MSE	MET	modified residue	UNP Q16666
B	134	MSE	MET	modified residue	UNP Q16666
B	156	MSE	MET	modified residue	UNP Q16666
B	188	MSE	MET	modified residue	UNP Q16666
B	195	MSE	MET	modified residue	UNP Q16666
C	1	GLY	-	cloning artifact	UNP Q16666

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	-	cloning artifact	UNP Q16666
C	3	HIS	-	cloning artifact	UNP Q16666
C	4	MSE	-	cloning artifact	UNP Q16666
C	36	MSE	MET	modified residue	UNP Q16666
C	41	MSE	MET	modified residue	UNP Q16666
C	134	MSE	MET	modified residue	UNP Q16666
C	156	MSE	MET	modified residue	UNP Q16666
C	188	MSE	MET	modified residue	UNP Q16666
C	195	MSE	MET	modified residue	UNP Q16666
D	1	GLY	-	cloning artifact	UNP Q16666
D	2	SER	-	cloning artifact	UNP Q16666
D	3	HIS	-	cloning artifact	UNP Q16666
D	4	MSE	-	cloning artifact	UNP Q16666
D	36	MSE	MET	modified residue	UNP Q16666
D	41	MSE	MET	modified residue	UNP Q16666
D	134	MSE	MET	modified residue	UNP Q16666
D	156	MSE	MET	modified residue	UNP Q16666
D	188	MSE	MET	modified residue	UNP Q16666
D	195	MSE	MET	modified residue	UNP Q16666

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	C	1	1	1	0	0

- Molecule 3 is water.

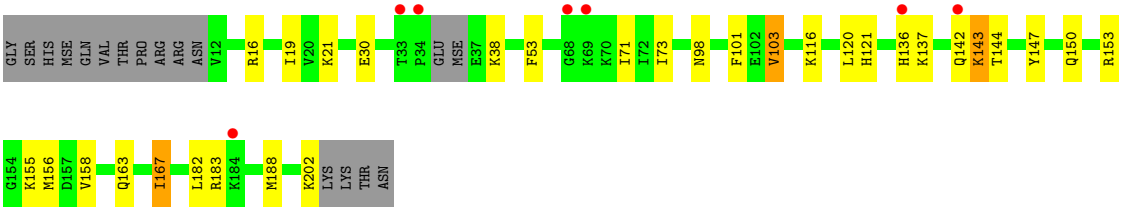
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	27	27	27	0	0
			Total	O		
3	B	45	45	45	0	0
			Total	O		
3	C	57	57	57	0	0
			Total	O		
3	D	30	30	30	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

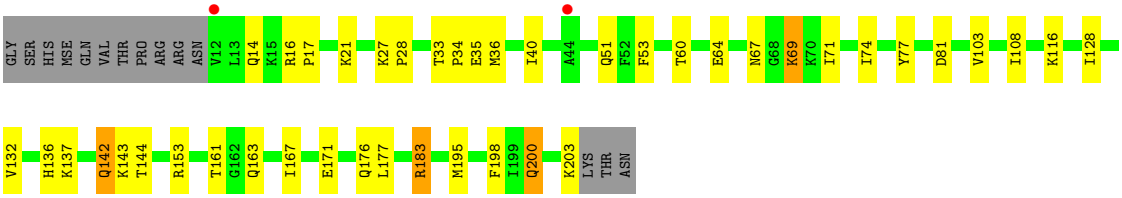
• Molecule 1: Gamma-interferon-inducible protein Ifi-16

Chain A:



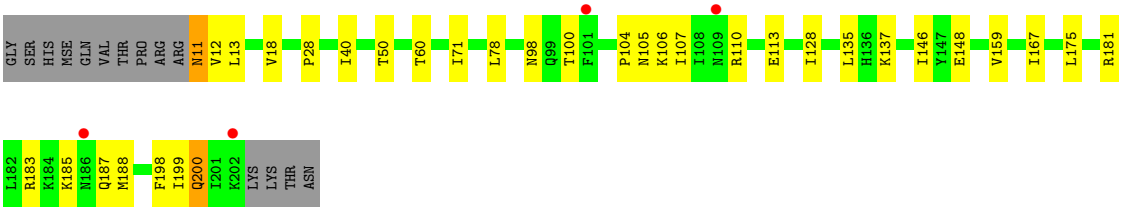
• Molecule 1: Gamma-interferon-inducible protein Ifi-16

Chain B:



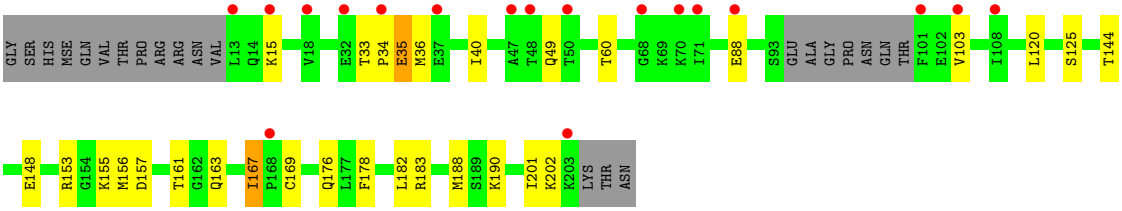
• Molecule 1: Gamma-interferon-inducible protein Ifi-16

Chain C:



• Molecule 1: Gamma-interferon-inducible protein Ifi-16

Chain D:


GLY SER HIS MSE GLN VAL THR PRO ARG ARG ASN VAL L13 Q14 K15 V18 E32 T33 P34 E35 M36 E37 I40 A47 T48 Q49 T50 T60 G68 K69 K70 I71 E88 S93 GLU ALA GLY PRO ASN GLN THR F101 E102 V103 I108 L120 S125 T144
E148 R153 G154 K155 M156 D157 T161 G162 Q163 I167 P168 C169 Q176 L177 F178 L182 R183 M188 S189 K190 I201 K202 K203 LYS THR ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.34Å 88.96Å 112.83Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	41.31 – 2.00 41.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (41.31-2.00) 96.4 (41.30-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.00Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.208 , 0.260 0.209 , 0.260	Depositor DCC
R_{free} test set	2783 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6320	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.47	0/1570	0.59	0/2099
1	B	0.57	0/1583	0.66	0/2114
1	C	0.62	0/1575	0.71	0/2106
1	D	0.51	0/1518	0.62	0/2024
All	All	0.55	0/6246	0.65	0/8343

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	A	1544	0	1601	19	0
1	B	1561	0	1620	31	0
1	C	1555	0	1602	15	0
1	D	1500	0	1557	13	0
2	C	1	0	0	0	0
3	A	27	0	0	1	0
3	B	45	0	0	0	0
3	C	57	0	0	0	0
3	D	30	0	0	1	0
All	All	6320	0	6380	70	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 6.

The worst 5 of 70 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:A:53:PHE:HE1	1:B:16:ARG:HD3	1.44	0.81
1:B:183:ARG:HH21	1:B:183:ARG:HG3	1.45	0.81
1:B:200:GLN:HE22	1:B:203:LYS:HE3	1.46	0.80
1:B:183:ARG:HH21	1:B:183:ARG:CG	2.00	0.74
1:A:53:PHE:CE1	1:B:16:ARG:HD3	2.23	0.73

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	187/206 (91%)	182 (97%)	5 (3%)	0	100	100
1	B	191/206 (93%)	183 (96%)	8 (4%)	0	100	100
1	C	190/206 (92%)	185 (97%)	5 (3%)	0	100	100
1	D	180/206 (87%)	171 (95%)	8 (4%)	1 (1%)	25	19
All	All	748/824 (91%)	721 (96%)	26 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	35	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	A	178/185 (96%)	167 (94%)	11 (6%)	18	13
1	B	180/185 (97%)	171 (95%)	9 (5%)	24	20
1	C	179/185 (97%)	166 (93%)	13 (7%)	14	9
1	D	173/185 (94%)	163 (94%)	10 (6%)	20	15
All	All	710/740 (96%)	667 (94%)	43 (6%)	19	14

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	105	ASN
1	D	49	GLN
1	C	183	ARG
1	C	200	GLN
1	D	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	GLN
1	B	200	GLN
1	D	200	GLN
1	D	123	GLN
1	A	165	HIS

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	184/206 (89%)	0.51	7 (3%)	40	39	42, 52, 61, 68	2 (1%)
1	B	186/206 (90%)	0.43	2 (1%)	80	79	36, 45, 56, 66	1 (0%)
1	C	186/206 (90%)	0.45	4 (2%)	62	60	33, 41, 55, 60	3 (1%)
1	D	178/206 (86%)	0.65	18 (10%)	7	6	39, 49, 61, 69	3 (1%)
All	All	734/824 (89%)	0.51	31 (4%)	36	35	33, 48, 59, 69	9 (1%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	ILE	5.0
1	D	15	LYS	4.9
1	D	13	LEU	4.5
1	D	70	LYS	4.5
1	D	50	THR	4.4

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	C	207	1/1	0.99	0.05	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.