wwPDB X-ray Structure Validation Summary Report (i)

Nov 27, 2024 – 04:08 PM JST

PDB ID	:	8Y31
Title	:	The crystal structure of the QX006N-Fab/IFNAR1-SD123 complex
Authors	:	Li, W.; Feng, W.
Deposited on	:	2024-01-28
Resolution	:	2.68 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:

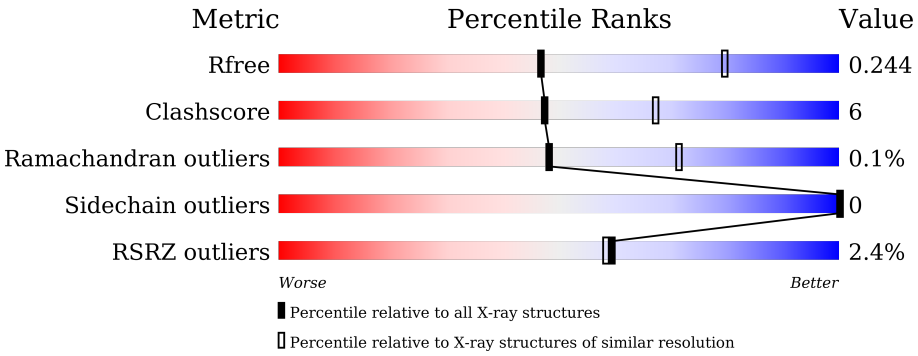
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.68 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}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	216	91% 9%
1	C	216	88% 12%
2	B	230	90% 6%
2	D	230	87% 9%
3	E	346	24% 5% 71%
3	F	346	23% 6% 71%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8330 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 QX006N-Fab-LC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1622	1011	271	335	5			
1	C	215	Total	C	N	O	S	0	0	0
			1622	1011	271	335	5			

- Molecule 2 is a protein called QX006N-Fab-HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1650	1045	274	324	7			
2	D	221	Total	C	N	O	S	0	0	0
			1650	1045	274	324	7			

- Molecule 3 is a protein called Interferon alpha/beta receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	102	Total	C	N	O	S	0	0	0
			859	554	143	159	3			
3	F	102	Total	C	N	O	S	0	0	0
			859	554	143	159	3			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	334	GLU	-	expression tag	UNP P17181
E	335	VAL	-	expression tag	UNP P17181
E	336	LEU	-	expression tag	UNP P17181
E	337	PHE	-	expression tag	UNP P17181
E	338	GLN	-	expression tag	UNP P17181
E	339	GLY	-	expression tag	UNP P17181
E	340	PRO	-	expression tag	UNP P17181
E	341	HIS	-	expression tag	UNP P17181

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Chain	Residue	Modelled	Actual	Comment	Reference
E	342	HIS	-	expression tag	UNP P17181
E	343	HIS	-	expression tag	UNP P17181
E	344	HIS	-	expression tag	UNP P17181
E	345	HIS	-	expression tag	UNP P17181
E	346	HIS	-	expression tag	UNP P17181
F	334	GLU	-	expression tag	UNP P17181
F	335	VAL	-	expression tag	UNP P17181
F	336	LEU	-	expression tag	UNP P17181
F	337	PHE	-	expression tag	UNP P17181
F	338	GLN	-	expression tag	UNP P17181
F	339	GLY	-	expression tag	UNP P17181
F	340	PRO	-	expression tag	UNP P17181
F	341	HIS	-	expression tag	UNP P17181
F	342	HIS	-	expression tag	UNP P17181
F	343	HIS	-	expression tag	UNP P17181
F	344	HIS	-	expression tag	UNP P17181
F	345	HIS	-	expression tag	UNP P17181
F	346	HIS	-	expression tag	UNP P17181

- Molecule 4 is water.

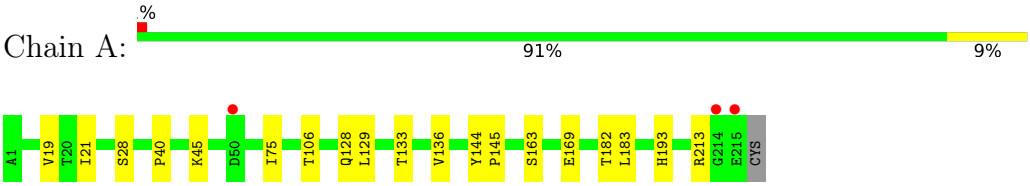
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	16	Total O 16 16	0	0
4	C	16	Total O 16 16	0	0
4	D	12	Total O 12 12	0	0
4	E	3	Total O 3 3	0	0
4	F	2	Total O 2 2	0	0

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.

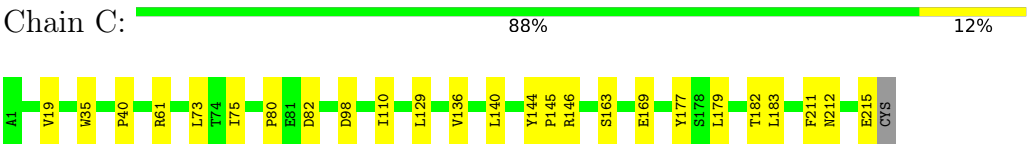
• Molecule 1: QX006N-Fab-LC

Chain A:



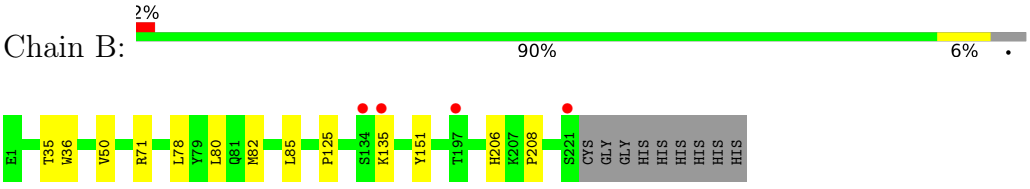
• Molecule 1: QX006N-Fab-LC

Chain C:



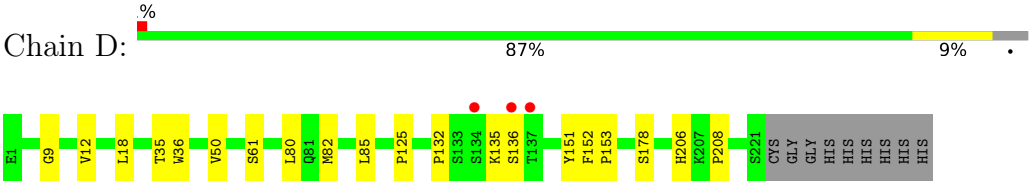
• Molecule 2: QX006N-Fab-HC

Chain B:



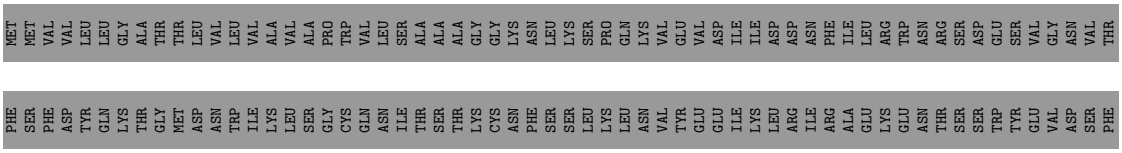
• Molecule 2: QX006N-Fab-HC

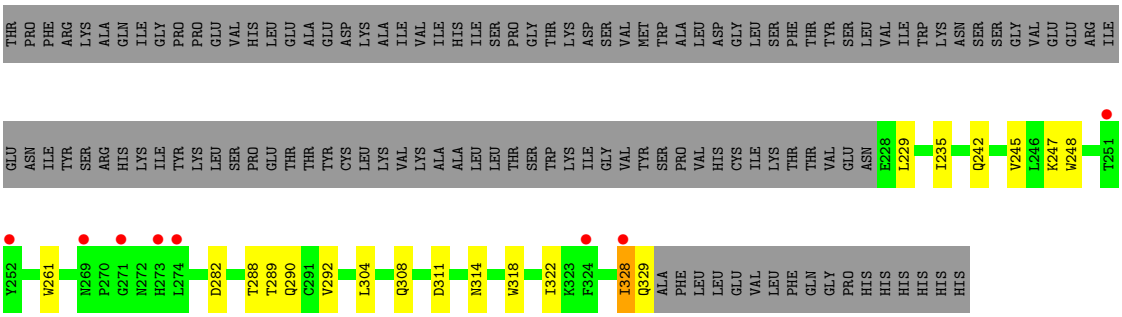
Chain D:



• Molecule 3: Interferon alpha/beta receptor 1

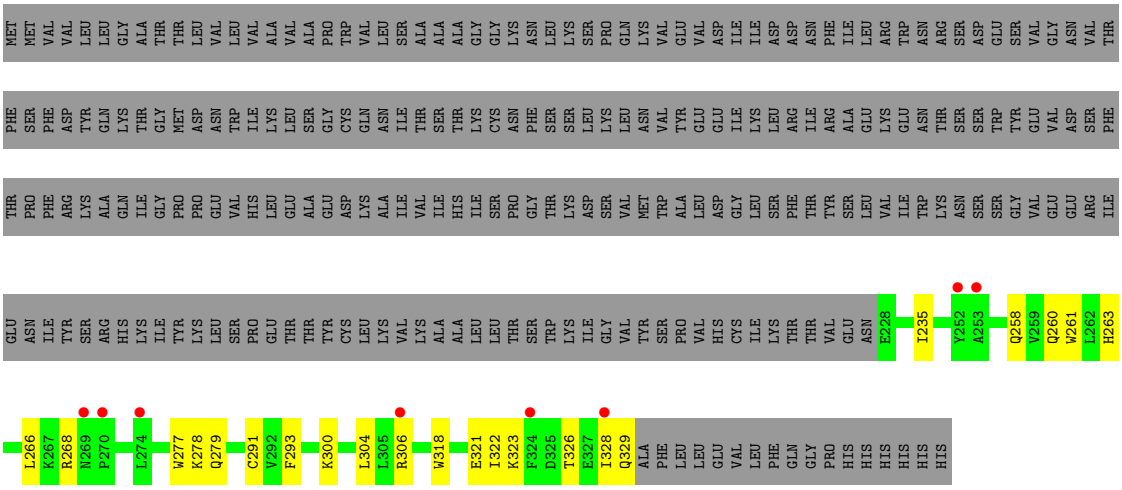
Chain E:





• Molecule 3: Interferon alpha/beta receptor 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.16Å 121.03Å 79.74Å 90.00° 111.51° 90.00°	Depositor
Resolution (Å)	46.89 – 2.68 46.89 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.89-2.68) 98.7 (46.89-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.194 , 0.239 0.199 , 0.244	Depositor DCC
R_{free} test set	1786 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8330	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

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	0.33	0/1652	0.56	0/2239
1	C	0.31	0/1652	0.54	0/2239
2	B	0.34	0/1689	0.56	0/2303
2	D	0.32	0/1689	0.54	0/2303
3	E	0.37	0/885	0.61	0/1206
3	F	0.32	0/885	0.53	0/1206
All	All	0.33	0/8452	0.55	0/11496

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	1622	0	1585	12	0
1	C	1622	0	1585	15	0
2	B	1650	0	1626	8	0
2	D	1650	0	1626	13	0
3	E	859	0	816	16	0
3	F	859	0	816	30	0
4	A	19	0	0	1	0
4	B	16	0	0	0	0
4	C	16	0	0	0	0
4	D	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	8330	0	8054	90	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 90 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)
3:F:277:TRP:CZ2	3:F:306:ARG:HD2	1.89	1.06
3:F:277:TRP:CH2	3:F:306:ARG:HD2	2.06	0.90
3:E:328:ILE:HG22	3:E:328:ILE:O	1.81	0.81
3:F:277:TRP:CH2	3:F:306:ARG:CD	2.65	0.79
3:E:328:ILE:O	3:E:328:ILE:CG2	2.35	0.74

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	213/216 (99%)	206 (97%)	7 (3%)	0	100 100
1	C	213/216 (99%)	206 (97%)	7 (3%)	0	100 100
2	B	219/230 (95%)	211 (96%)	8 (4%)	0	100 100
2	D	219/230 (95%)	213 (97%)	6 (3%)	0	100 100
3	E	100/346 (29%)	94 (94%)	5 (5%)	1 (1%)	13 29
3	F	100/346 (29%)	95 (95%)	5 (5%)	0	100 100
All	All	1064/1584 (67%)	1025 (96%)	38 (4%)	1 (0%)	48 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	328	ILE

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	183/184 (100%)	183 (100%)	0	100	100
1	C	183/184 (100%)	183 (100%)	0	100	100
2	B	184/191 (96%)	184 (100%)	0	100	100
2	D	184/191 (96%)	184 (100%)	0	100	100
3	E	96/314 (31%)	96 (100%)	0	100	100
3	F	96/314 (31%)	96 (100%)	0	100	100
All	All	926/1378 (67%)	926 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	260	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	215/216 (99%)	-0.15	3 (1%) 73 72	30, 51, 66, 79	0
1	C	215/216 (99%)	-0.17	0 100 100	34, 52, 69, 98	0
2	B	221/230 (96%)	-0.20	4 (1%) 67 67	32, 46, 80, 98	0
2	D	221/230 (96%)	-0.16	3 (1%) 73 72	33, 48, 77, 92	0
3	E	102/346 (29%)	0.54	8 (7%) 20 19	46, 72, 95, 112	0
3	F	102/346 (29%)	0.67	8 (7%) 20 19	46, 75, 99, 102	0
All	All	1076/1584 (67%)	-0.02	26 (2%) 59 58	30, 52, 87, 112	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	GLU	4.2
1	A	214	GLY	3.6
2	D	136	SER	3.1
3	E	328	ILE	3.1
3	F	324	PHE	3.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.