wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2021 – 09:16 AM EDT

PDB ID	:	1Y6N
Title	:	Crystal structure of Epstein-Barr virus IL-10 mutant (A87I) complexed with the soluble IL-10R1 chain
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Deposited on	:	2004-12-06
Resolution	:	2.70 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 following versions of software and data (see references (1)) were used in the production of this report:

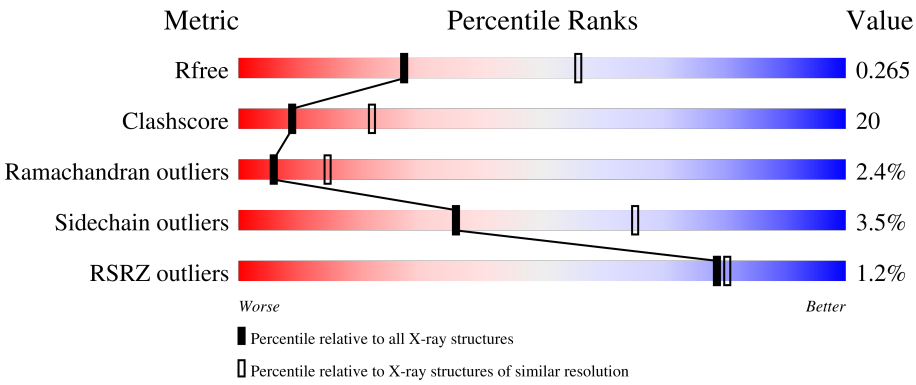
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	L	145	3% 58% 38% • •
2	R	214	60% 31% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2846 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 Viral interleukin-10 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	L	142	1179	750	200	220	4	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	22	MSE	MET	modified residue	UNP P03180
L	68	MSE	MET	modified residue	UNP P03180
L	77	MSE	MET	modified residue	UNP P03180
L	87	ILE	ALA	engineered mutation	UNP P03180
L	140	MSE	MET	modified residue	UNP P03180
L	154	MSE	MET	modified residue	UNP P03180

- Molecule 2 is a protein called Interleukin-10 receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	R	202	1626	1036	280	304	6	4	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	29	GLN	ASN	engineered mutation	UNP Q13651
R	53	GLN	ASN	engineered mutation	UNP Q13651
R	89	GLN	ASN	engineered mutation	UNP Q13651
R	133	GLN	ASN	engineered mutation	UNP Q13651
R	156	GLN	ASN	engineered mutation	UNP Q13651
R	168	GLN	ASN	engineered mutation	UNP Q13651

- Molecule 3 is water.

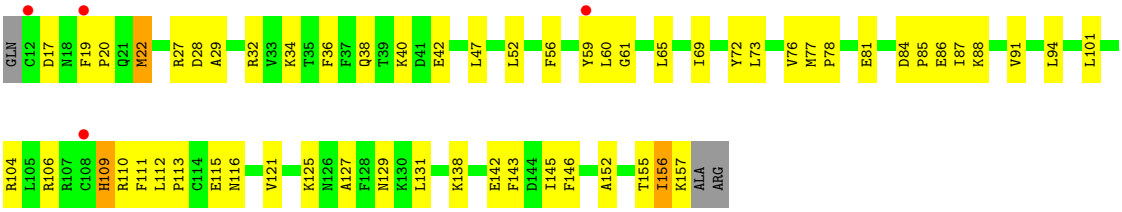
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	L	7	7	7	0	0
			Total	O		
3	R	34	34	34	0	0

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.

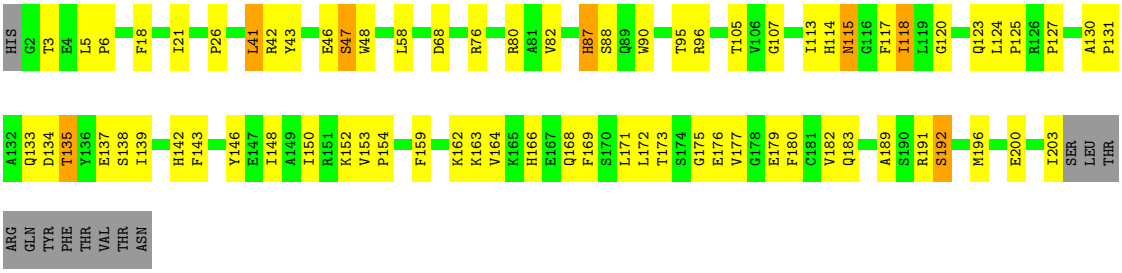
• Molecule 1: Viral interleukin-10 homolog

Chain L:



• Molecule 2: Interleukin-10 receptor alpha chain

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	45.60Å 45.60Å 310.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.70 51.77 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.70) 91.8 (51.77-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.58Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.271 0.207 , 0.265	Depositor DCC
R_{free} test set	820 reflections (7.27%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.100 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2846	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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)

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	L	0.37	0/1194	0.57	0/1591
2	R	0.40	0/1672	0.69	0/2272
All	All	0.39	0/2866	0.64	0/3863

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	L	1179	0	1173	45	0
2	R	1626	0	1569	70	0
3	L	7	0	0	2	0
3	R	34	0	0	0	0
All	All	2846	0	2742	113	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 20.

The worst 5 of 113 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:R:135:THR:HG22	2:R:138:SER:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:191:ARG:HH11	2:R:191:ARG:HG3	1.39	0.87
2:R:105:THR:HG22	2:R:196:MET:HB3	1.60	0.82
1:L:36:PHE:O	1:L:40:LYS:HD3	1.82	0.80
2:R:118:ILE:HG13	2:R:171:LEU:HB2	1.65	0.79

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	L	140/145 (97%)	122 (87%)	14 (10%)	4 (3%)	4 10
2	R	200/214 (94%)	185 (92%)	11 (6%)	4 (2%)	7 19
All	All	340/359 (95%)	307 (90%)	25 (7%)	8 (2%)	6 15

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	110	ARG
1	L	109	HIS
2	R	176	GLU
1	L	17	ASP
2	R	47	SER

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	L	131/128 (102%)	128 (98%)	3 (2%)	50	78
2	R	182/194 (94%)	174 (96%)	8 (4%)	28	56
All	All	313/322 (97%)	302 (96%)	11 (4%)	36	65

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	135	THR
2	R	172	LEU
2	R	200	GLU
2	R	192	SER
2	R	87	HIS

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

Mol	Chain	Res	Type
2	R	110	ASN
2	R	123	GLN
2	R	183	GLN
2	R	166	HIS
2	R	168	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)

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	L	137/145 (94%)	-0.13	4 (2%) 51 52	24, 51, 79, 93	0
2	R	202/214 (94%)	-0.43	0 100 100	16, 34, 64, 82	1 (0%)
All	All	339/359 (94%)	-0.31	4 (1%) 79 80	16, 39, 75, 93	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	12	CYS	3.1
1	L	108	CYS	2.7
1	L	19	PHE	2.2
1	L	59	TYR	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.