Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2024 – 12:44 am GMT

PDB ID	:	8ODX
Title	:	Interleukin 12 receptor subunit beta-1 Fn domains in complex with antagonistic FAb4 fragment and VHH.
Authors	:	Bloch, Y.; Savvides, S.N.
Deposited on	:	2023-03-09
Resolution	:	4.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

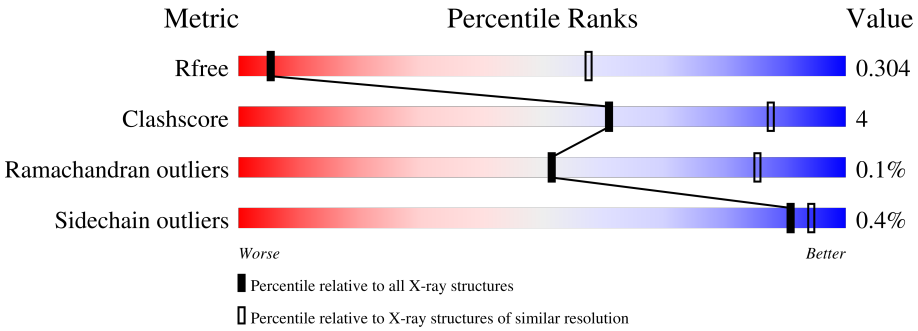
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)

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	A	376	64% 11% 25%
2	H	250	82% 6% 12%
3	K	167	63% 8% • 28%
4	L	231	85% 7% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6382 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 Interleukin-12 receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2175	1365	385	412	13	0	0	0

There are 67 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MET	-	initiating methionine	UNP P42701
A	204	GLY	-	expression tag	UNP P42701
A	205	ILE	-	expression tag	UNP P42701
A	206	LEU	-	expression tag	UNP P42701
A	207	PRO	-	expression tag	UNP P42701
A	208	SER	-	expression tag	UNP P42701
A	209	PRO	-	expression tag	UNP P42701
A	210	GLY	-	expression tag	UNP P42701
A	211	MET	-	expression tag	UNP P42701
A	212	PRO	-	expression tag	UNP P42701
A	213	ALA	-	expression tag	UNP P42701
A	214	LEU	-	expression tag	UNP P42701
A	215	LEU	-	expression tag	UNP P42701
A	216	SER	-	expression tag	UNP P42701
A	217	LEU	-	expression tag	UNP P42701
A	218	VAL	-	expression tag	UNP P42701
A	219	SER	-	expression tag	UNP P42701
A	220	LEU	-	expression tag	UNP P42701
A	221	LEU	-	expression tag	UNP P42701
A	222	SER	-	expression tag	UNP P42701
A	223	VAL	-	expression tag	UNP P42701
A	224	LEU	-	expression tag	UNP P42701
A	225	LEU	-	expression tag	UNP P42701
A	226	MET	-	expression tag	UNP P42701
A	227	GLY	-	expression tag	UNP P42701
A	228	CYS	-	expression tag	UNP P42701
A	229	VAL	-	expression tag	UNP P42701

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	ALA	-	expression tag	UNP P42701
A	231	GLU	-	expression tag	UNP P42701
A	541	GLY	-	expression tag	UNP P42701
A	542	THR	-	expression tag	UNP P42701
A	543	SER	-	expression tag	UNP P42701
A	544	ASP	-	expression tag	UNP P42701
A	545	GLU	-	expression tag	UNP P42701
A	546	VAL	-	expression tag	UNP P42701
A	547	ASP	-	expression tag	UNP P42701
A	548	GLY	-	expression tag	UNP P42701
A	549	GLY	-	expression tag	UNP P42701
A	550	SER	-	expression tag	UNP P42701
A	551	GLY	-	expression tag	UNP P42701
A	552	GLY	-	expression tag	UNP P42701
A	553	SER	-	expression tag	UNP P42701
A	554	GLY	-	expression tag	UNP P42701
A	555	LEU	-	expression tag	UNP P42701
A	556	ASN	-	expression tag	UNP P42701
A	557	ASP	-	expression tag	UNP P42701
A	558	ILE	-	expression tag	UNP P42701
A	559	PHE	-	expression tag	UNP P42701
A	560	GLU	-	expression tag	UNP P42701
A	561	ALA	-	expression tag	UNP P42701
A	562	GLN	-	expression tag	UNP P42701
A	563	LYS	-	expression tag	UNP P42701
A	564	ILE	-	expression tag	UNP P42701
A	565	GLU	-	expression tag	UNP P42701
A	566	TRP	-	expression tag	UNP P42701
A	567	HIS	-	expression tag	UNP P42701
A	568	GLU	-	expression tag	UNP P42701
A	569	GLY	-	expression tag	UNP P42701
A	570	ARG	-	expression tag	UNP P42701
A	571	THR	-	expression tag	UNP P42701
A	572	LYS	-	expression tag	UNP P42701
A	573	HIS	-	expression tag	UNP P42701
A	574	HIS	-	expression tag	UNP P42701
A	575	HIS	-	expression tag	UNP P42701
A	576	HIS	-	expression tag	UNP P42701
A	577	HIS	-	expression tag	UNP P42701
A	578	HIS	-	expression tag	UNP P42701

- Molecule 2 is a protein called FAb4 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1646	1036	276	328	6			

- Molecule 3 is a protein called anti Kappa Light chain VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	120	Total	C	N	O	S	0	0	0
			921	571	162	184	4			

- Molecule 4 is a protein called FAb4 Light chain.

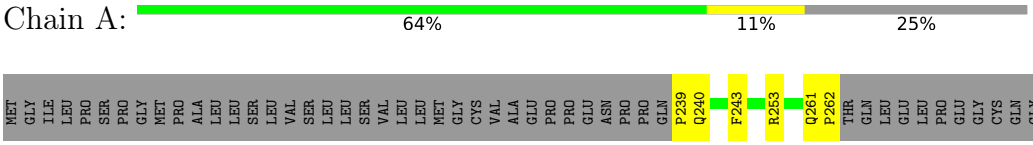
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1640	1032	272	331	5			

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.

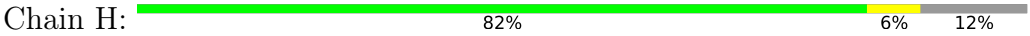
- Molecule 1: Interleukin-12 receptor subunit beta-1

Chain A:



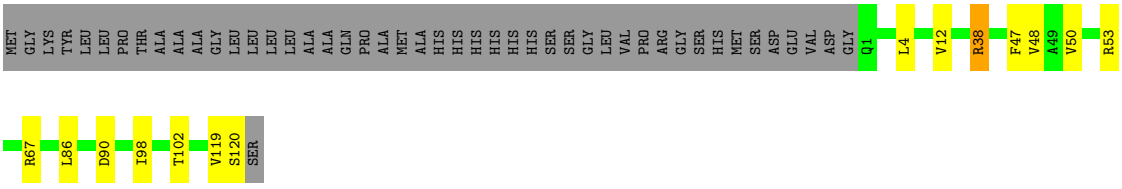
- Molecule 2: FAb4 Heavy chain

Chain H:



- Molecule 3: anti Kappa Light chain VHH

Chain K:



- Molecule 4: FAb4 Light chain

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	231.40Å 231.40Å 231.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.81 – 4.40 163.63 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (81.81-4.40) 100.0 (163.63-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 4.47Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.280 , 0.311 0.273 , 0.304	Depositor DCC
R_{free} test set	1398 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	246.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 297.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6382	wwPDB-VP
Average B, all atoms (Å^2)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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	0/2232	0.62	1/3045 (0.0%)
2	H	0.26	0/1686	0.51	0/2300
3	K	0.37	0/940	0.67	1/1272 (0.1%)
4	L	0.28	0/1679	0.50	0/2281
All	All	0.31	0/6537	0.57	2/8898 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	LEU	N-CA-CB	6.27	122.95	110.40
3	K	38	ARG	CB-CG-CD	5.57	126.08	111.60

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	2175	0	2111	32	0
2	H	1646	0	1589	7	0
3	K	921	0	862	10	0
4	L	1640	0	1584	10	0
All	All	6382	0	6146	56	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 4.

All (56) 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:320:SER:O	1:A:327:GLY:HA3	1.87	0.75
3:K:53:ARG:NH2	3:K:102:THR:O	2.27	0.67
3:K:38:ARG:NH2	3:K:90:ASP:HA	2.10	0.66
1:A:284:LEU:HB2	1:A:303:LEU:HD23	1.78	0.65
2:H:30:THR:HG22	2:H:74:ASN:HB3	1.79	0.65
3:K:67:ARG:NH2	3:K:90:ASP:OD2	2.30	0.65
3:K:12:VAL:HG11	3:K:86:LEU:HD13	1.79	0.64
4:L:145:VAL:HG22	4:L:195:VAL:HG22	1.78	0.64
1:A:282:TYR:HB3	1:A:303:LEU:CD1	2.30	0.62
3:K:38:ARG:HD2	3:K:48:VAL:HG22	1.83	0.61
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.85	0.58
3:K:38:ARG:HH21	3:K:90:ASP:HA	1.70	0.57
1:A:349:VAL:HA	1:A:354:THR:HG22	1.86	0.57
1:A:281:THR:HB	1:A:321:SER:HB3	1.85	0.57
1:A:282:TYR:HB3	1:A:303:LEU:HD11	1.86	0.57
1:A:240:GLN:HB3	1:A:262:PRO:HA	1.87	0.56
1:A:285:GLN:HB2	1:A:319:ILE:HD11	1.87	0.56
1:A:300:THR:HG22	4:L:91:TRP:HH2	1.70	0.54
1:A:318:VAL:O	1:A:329:ASN:HA	2.08	0.54
1:A:300:THR:HG22	4:L:91:TRP:CH2	2.43	0.53
4:L:145:VAL:HA	4:L:194:GLU:O	2.10	0.52
1:A:317:ALA:HA	1:A:330:GLN:O	2.10	0.52
3:K:119:VAL:O	3:K:120:SER:HB3	2.11	0.51
1:A:243:PHE:HB2	1:A:332:TRP:CE3	2.45	0.51
1:A:351:THR:O	1:A:403:ARG:HD3	2.12	0.50
1:A:481:TYR:HB2	1:A:498:VAL:HB	1.93	0.49
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.94	0.49
1:A:253:ARG:NH2	1:A:308:TYR:HB2	2.27	0.48
1:A:282:TYR:CB	1:A:303:LEU:HD12	2.43	0.48
1:A:282:TYR:HB3	1:A:303:LEU:HD12	1.96	0.47
1:A:243:PHE:HB2	1:A:332:TRP:CZ3	2.50	0.47
1:A:405:SER:O	1:A:407:ALA:N	2.48	0.47
1:A:240:GLN:HB3	1:A:261:GLN:O	2.15	0.46
1:A:239:PRO:HA	1:A:262:PRO:HB3	1.96	0.46
3:K:4:LEU:HD11	3:K:98:ILE:HG13	1.98	0.46
1:A:345:LEU:HD11	1:A:434:LEU:HD11	1.97	0.45
4:L:155:SER:C	4:L:157:ASN:H	2.20	0.45
4:L:36:GLN:HB2	4:L:46:LEU:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:SER:HB3	2:H:57:ASP:HB2	2.00	0.43
1:A:300:THR:O	4:L:91:TRP:HZ3	2.02	0.43
1:A:379:GLY:O	1:A:381:ALA:N	2.51	0.43
1:A:354:THR:HG21	1:A:407:ALA:O	2.19	0.43
1:A:405:SER:C	1:A:407:ALA:H	2.23	0.42
2:H:91:THR:HG23	2:H:118:THR:HA	2.01	0.42
1:A:408:MET:HG2	1:A:414:TYR:CG	2.55	0.42
1:A:282:TYR:HD1	1:A:320:SER:HG	1.66	0.41
3:K:47:PHE:HZ	3:K:50:VAL:HG12	1.85	0.41
3:K:53:ARG:HH21	3:K:102:THR:HB	1.84	0.41
4:L:88:GLN:HB2	4:L:97:PHE:CD1	2.56	0.41
1:A:408:MET:HA	1:A:414:TYR:CZ	2.55	0.41
1:A:484:ARG:O	1:A:518:VAL:HA	2.20	0.41
2:H:171:VAL:HG22	2:H:190:VAL:HG22	2.02	0.41
2:H:6:GLU:CD	2:H:114:GLY:H	2.24	0.41
1:A:290:SER:HB2	1:A:312:ALA:HB1	2.02	0.40
4:L:112:PRO:HB3	4:L:138:PHE:HB3	2.03	0.40
4:L:147:TRP:HB2	4:L:154:GLN:HB2	2.04	0.40

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	276/376 (73%)	265 (96%)	10 (4%)	1 (0%)	34 72
2	H	218/250 (87%)	206 (94%)	12 (6%)	0	100 100
3	K	118/167 (71%)	112 (95%)	6 (5%)	0	100 100
4	L	210/231 (91%)	201 (96%)	9 (4%)	0	100 100
All	All	822/1024 (80%)	784 (95%)	37 (4%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	LEU

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	238/314 (76%)	238 (100%)	0	100 100
2	H	183/209 (88%)	182 (100%)	1 (0%)	88 93
3	K	95/131 (72%)	95 (100%)	0	100 100
4	L	186/199 (94%)	184 (99%)	2 (1%)	73 85
All	All	702/853 (82%)	699 (100%)	3 (0%)	91 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	113	ARG
4	L	77	LEU
4	L	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
3	K	5	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

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.