



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 PM GMT

PDB ID : 4NN6
Title : Cytokine receptor complex - Crystal form 1B
Authors : Verstraete, K.; van Schie, L.; Savvides, S.N.
Deposited on : 2013-11-16
Resolution : 2.54 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

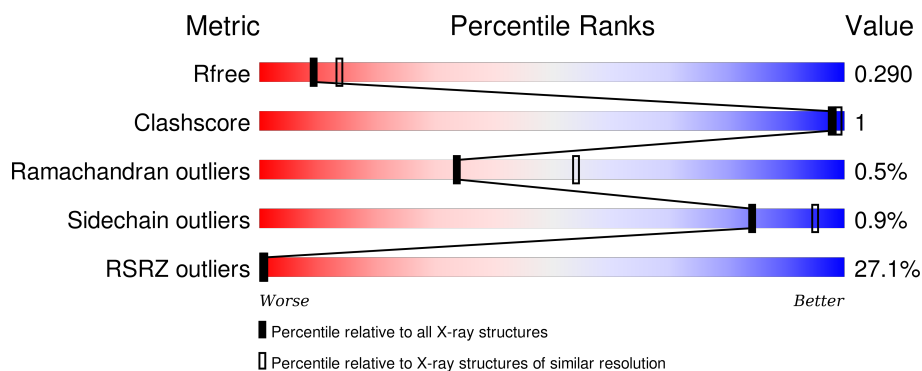
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	130	<div> <div>23%</div> <div>74%</div> <div>22%</div> </div>
2	B	223	<div> <div>16%</div> <div>83%</div> <div>13%</div> </div>
3	C	212	<div> <div>27%</div> <div>75%</div> <div>23%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6390 atoms, of which 3025 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 Thymic stromal lymphopoietin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	101	Total	C	H	N	O	S	0	0	0
			1377	467	644	120	138	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLN	ASN	ENGINEERED MUTATION	UNP Q9JIE6
A	141	GLY	-	EXPRESSION TAG	UNP Q9JIE6
A	142	THR	-	EXPRESSION TAG	UNP Q9JIE6
A	143	LYS	-	EXPRESSION TAG	UNP Q9JIE6
A	144	HIS	-	EXPRESSION TAG	UNP Q9JIE6
A	145	HIS	-	EXPRESSION TAG	UNP Q9JIE6
A	146	HIS	-	EXPRESSION TAG	UNP Q9JIE6
A	147	HIS	-	EXPRESSION TAG	UNP Q9JIE6
A	148	HIS	-	EXPRESSION TAG	UNP Q9JIE6
A	149	HIS	-	EXPRESSION TAG	UNP Q9JIE6

- Molecule 2 is a protein called Interleukin-7 receptor subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	193	Total	C	H	N	O	S	0	0	0
			2813	949	1353	249	254	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	GLY	-	EXPRESSION TAG	UNP P16872
B	18	SER	-	EXPRESSION TAG	UNP P16872
B	19	HIS	-	EXPRESSION TAG	UNP P16872
B	20	MET	-	EXPRESSION TAG	UNP P16872

- Molecule 3 is a protein called Cytokine receptor-like factor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	163	Total	C	H	N	O	S	0	0	0
			2197	735	1028	207	221	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	GLN	ASN	ENGINEERED MUTATION	UNP Q8CII9
C	179	VAL	ALA	CONFLICT	UNP Q8CII9
C	223	GLY	-	EXPRESSION TAG	UNP Q8CII9
C	224	THR	-	EXPRESSION TAG	UNP Q8CII9
C	225	LYS	-	EXPRESSION TAG	UNP Q8CII9
C	226	HIS	-	EXPRESSION TAG	UNP Q8CII9
C	227	HIS	-	EXPRESSION TAG	UNP Q8CII9
C	228	HIS	-	EXPRESSION TAG	UNP Q8CII9
C	229	HIS	-	EXPRESSION TAG	UNP Q8CII9
C	230	HIS	-	EXPRESSION TAG	UNP Q8CII9
C	231	HIS	-	EXPRESSION TAG	UNP Q8CII9

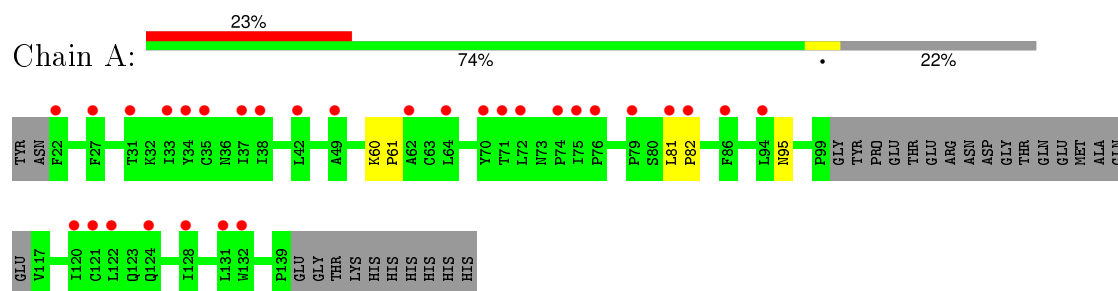
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		

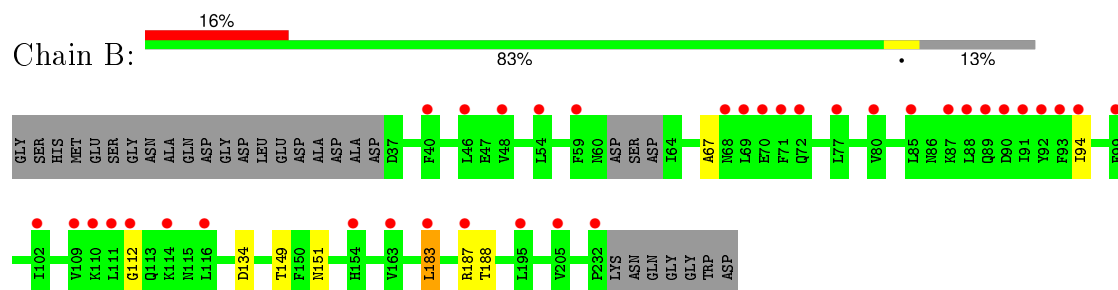
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

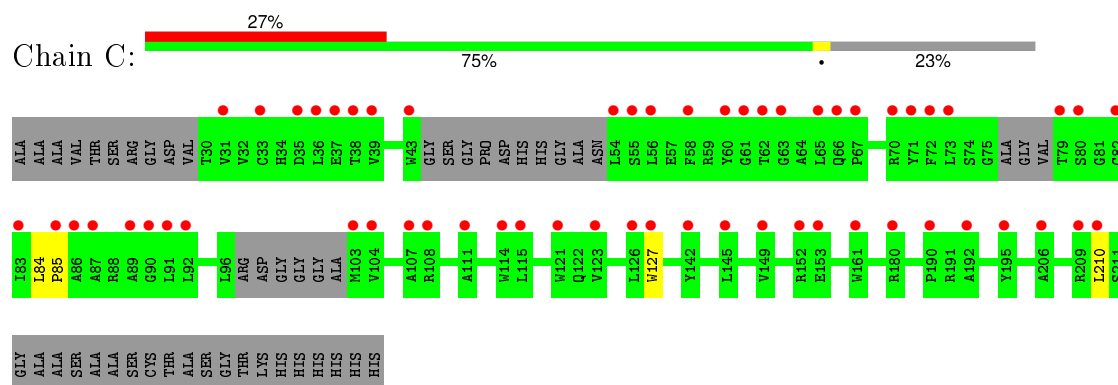
• Molecule 1: Thymic stromal lymphopoietin



• Molecule 2: Interleukin-7 receptor subunit alpha



• Molecule 3: Cytokine receptor-like factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.95Å 75.16Å 51.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.45 – 2.54 42.45 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.45-2.54) 99.6 (42.45-2.54)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.259 , 0.297 0.256 , 0.290	Depositor DCC
R_{free} test set	979 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 65.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19440 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6390	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.21	0/750	0.38	0/1026
2	B	0.24	0/1500	0.45	0/2046
3	C	0.23	0/1199	0.48	0/1651
All	All	0.23	0/3449	0.45	0/4723

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	733	644	646	2	0
2	B	1460	1353	1363	3	0
3	C	1169	1028	1032	2	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
All	All	3365	3025	3041	7	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 1.

All (7) 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:B:149:THR:HG22	2:B:187:ARG:HG2	1.88	0.56
2:B:134:ASP:OD2	2:B:151:ASN:ND2	2.41	0.51
3:C:84:LEU:HB2	3:C:85:PRO:HD2	2.00	0.43
1:A:81:LEU:HB3	1:A:82:PRO:HD3	2.00	0.43
2:B:183:LEU:HD21	2:B:188:THR:HB	2.01	0.43
1:A:60:LYS:N	1:A:61:PRO:HD2	2.36	0.41
3:C:127:TRP:NE1	3:C:210:LEU:HD21	2.37	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	97/130 (75%)	95 (98%)	2 (2%)	0	100	100
2	B	189/223 (85%)	181 (96%)	6 (3%)	2 (1%)	17	30
3	C	155/212 (73%)	154 (99%)	1 (1%)	0	100	100
All	All	441/565 (78%)	430 (98%)	9 (2%)	2 (0%)	34	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	67	ALA
2	B	112	GLY

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	73/119 (61%)	72 (99%)	1 (1%)	74	90
2	B	144/198 (73%)	142 (99%)	2 (1%)	74	90
3	C	109/165 (66%)	109 (100%)	0	100	100
All	All	326/482 (68%)	323 (99%)	3 (1%)	84	95

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

Mol	Chain	Res	Type
1	A	95	ASN
2	B	94	ILE
2	B	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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, 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	101/130 (77%)	1.57	30 (29%) 1 0	50, 103, 146, 158	0
2	B	193/223 (86%)	1.28	36 (18%) 2 2	45, 70, 138, 193	0
3	C	163/212 (76%)	1.78	58 (35%) 0 0	53, 84, 163, 193	0
All	All	457/565 (80%)	1.52	124 (27%) 1 0	45, 83, 155, 193	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	114	TRP	8.8
2	B	92	TYR	8.6
1	A	81	LEU	7.5
2	B	87	LYS	6.6
2	B	88	LEU	6.5
3	C	72	PHE	6.4
1	A	128	ILE	6.3
2	B	111	LEU	6.1
3	C	91	LEU	5.9
3	C	62	THR	5.8
1	A	72	LEU	5.8
3	C	55	SER	5.7
2	B	91	ILE	5.7
3	C	111	ALA	5.7
1	A	75	ILE	5.5
2	B	90	ASP	5.4
3	C	71	TYR	5.3
3	C	66	GLN	5.2
1	A	74	PRO	5.2
3	C	115	LEU	5.1
3	C	65	LEU	4.8
3	C	36	LEU	4.7
3	C	61	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
3	C	85	PRO	4.6
1	A	132	TRP	4.6
2	B	68	ASN	4.6
1	A	70	TYR	4.5
2	B	59	PHE	4.4
1	A	79	PRO	4.4
3	C	54	LEU	4.3
3	C	92	LEU	4.3
3	C	86	ALA	4.3
2	B	70	GLU	4.2
3	C	31	VAL	4.2
2	B	69	LEU	4.2
3	C	67	PRO	4.1
3	C	190	PRO	4.1
3	C	43	TRP	4.0
3	C	104	VAL	4.0
1	A	76	PRO	3.9
2	B	110	LYS	3.9
3	C	33	CYS	3.9
3	C	56	LEU	3.8
3	C	145	LEU	3.8
1	A	71	THR	3.8
2	B	71	PHE	3.8
2	B	85	LEU	3.7
2	B	109	VAL	3.7
3	C	209	ARG	3.7
1	A	49	ALA	3.7
3	C	153	GLU	3.6
1	A	131	LEU	3.6
3	C	121	TRP	3.5
2	B	48	VAL	3.4
1	A	34	TYR	3.3
3	C	58	PHE	3.2
2	B	116	LEU	3.2
2	B	93	PHE	3.1
3	C	37	GLU	3.1
2	B	232	PRO	3.0
3	C	79	THR	3.0
1	A	42	LEU	3.0
1	A	37	ILE	2.9
3	C	39	VAL	2.8
3	C	123	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	38	THR	2.8
1	A	121	CYS	2.8
1	A	64	LEU	2.8
3	C	103	MET	2.8
3	C	87	ALA	2.8
3	C	195	TYR	2.8
1	A	94	LEU	2.7
3	C	63	GLY	2.7
2	B	114	LYS	2.7
3	C	60	TYR	2.7
2	B	54	LEU	2.7
3	C	73	LEU	2.7
3	C	80	SER	2.7
1	A	120	ILE	2.7
1	A	27	PHE	2.7
1	A	38	ILE	2.6
1	A	82	PRO	2.6
3	C	210	LEU	2.6
1	A	22	PHE	2.6
2	B	94	ILE	2.6
1	A	33	ILE	2.5
2	B	112	GLY	2.5
2	B	154	HIS	2.5
3	C	192	ALA	2.5
2	B	89	GLN	2.5
1	A	31	THR	2.4
1	A	62	ALA	2.4
3	C	70	ARG	2.4
2	B	183	LEU	2.4
3	C	142	TYR	2.4
3	C	152	ARG	2.4
3	C	127	TRP	2.4
3	C	108	ARG	2.3
1	A	35	CYS	2.3
2	B	205	VAL	2.3
3	C	82	CYS	2.3
2	B	102	ILE	2.3
2	B	99	PHE	2.3
2	B	195	LEU	2.3
3	C	180	ARG	2.3
3	C	149	VAL	2.2
2	B	72	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	89	ALA	2.2
3	C	83	ILE	2.2
3	C	35	ASP	2.2
3	C	126	LEU	2.2
1	A	124	GLN	2.2
2	B	187	ARG	2.2
2	B	163	VAL	2.1
2	B	40	PHE	2.1
3	C	107	ALA	2.1
1	A	86	PHE	2.1
1	A	122	LEU	2.1
3	C	206	ALA	2.1
3	C	161	TRP	2.1
2	B	77	LEU	2.0
3	C	90	GLY	2.0
2	B	80	VAL	2.0
2	B	46	LEU	2.0

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 carbohydrates 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.