



Full wwPDB X-ray Structure Validation Report

Feb 22, 2018 – 01:06 AM EST

PDB ID : 5J12
Title : Structure of human TSLP:TSLPR in complex with mouse IL-7Ralpha
Authors : Verstraete, K.; Savvides, S.N.
Deposited on : 2016-03-28
Resolution : 3.55 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

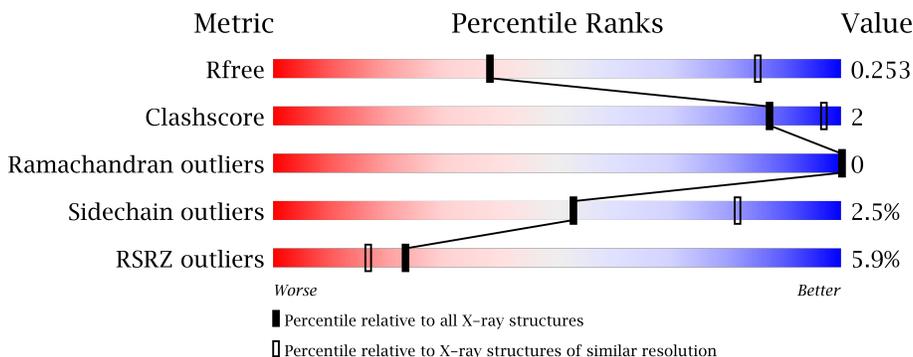
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	100719	1072 (3.70-3.42)
Clashscore	112137	1003 (3.66-3.46)
Ramachandran outliers	110173	1153 (3.70-3.42)
Sidechain outliers	110143	1153 (3.70-3.42)
RSRZ outliers	101464	1098 (3.70-3.42)

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	163	 .% 68% 10% 22%
2	B	223	 9% 82% 5% 13%
3	C	230	 4% 77% 6% 18%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3819 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 Thymic stromal lymphopoietin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	977	613	168	187	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLN	ASN	engineered mutation	UNP Q969D9
A	?	-	LYS	deletion	UNP Q969D9
A	?	-	ARG	deletion	UNP Q969D9
A	?	-	ARG	deletion	UNP Q969D9
A	?	-	LYS	deletion	UNP Q969D9
A	?	-	ARG	deletion	UNP Q969D9
A	131	SER	LYS	engineered mutation	UNP Q969D9
A	160	GLY	-	expression tag	UNP Q969D9
A	161	THR	-	expression tag	UNP Q969D9
A	162	LYS	-	expression tag	UNP Q969D9
A	163	HIS	-	expression tag	UNP Q969D9
A	164	HIS	-	expression tag	UNP Q969D9
A	165	HIS	-	expression tag	UNP Q969D9
A	166	HIS	-	expression tag	UNP Q969D9
A	167	HIS	-	expression tag	UNP Q969D9
A	168	HIS	-	expression tag	UNP Q969D9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	194	1355	871	229	248	7	0	0	0

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

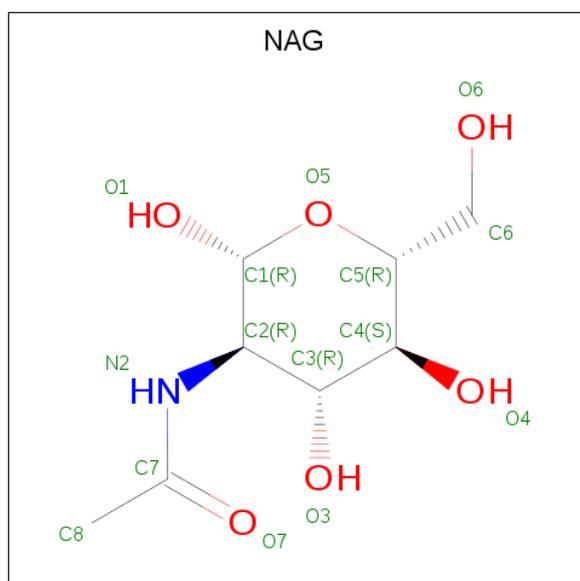
- Molecule 3 is a protein called Cytokine receptor-like factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	189	1425	914	228	274	9	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

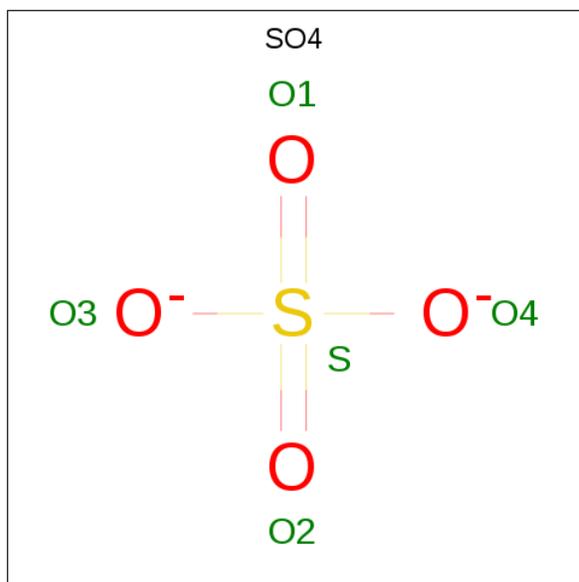
Chain	Residue	Modelled	Actual	Comment	Reference
C	222	GLY	-	expression tag	UNP Q9HC73
C	223	THR	-	expression tag	UNP Q9HC73
C	224	LYS	-	expression tag	UNP Q9HC73
C	225	HIS	-	expression tag	UNP Q9HC73
C	226	HIS	-	expression tag	UNP Q9HC73
C	227	HIS	-	expression tag	UNP Q9HC73
C	228	HIS	-	expression tag	UNP Q9HC73
C	229	HIS	-	expression tag	UNP Q9HC73
C	230	HIS	-	expression tag	UNP Q9HC73

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	O	0	0
			3	3		
6	C	2	Total	O	0	0
			2	2		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.44Å 125.44Å 194.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.43 – 3.55 47.43 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.43-3.55) 98.5 (47.43-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.57Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.214 , 0.225 0.233 , 0.253	Depositor DCC
R_{free} test set	567 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	125.2	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 133.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3819	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAG, SO4

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	0.65	0/998	0.78	0/1355
2	B	0.48	0/1388	0.65	1/1911 (0.1%)
3	C	0.51	0/1467	0.73	0/2018
All	All	0.54	0/3853	0.71	1/5284 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	HIS	C-N-CA	5.91	136.48	121.70

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	977	0	906	9	0
2	B	1355	0	1161	8	0
3	C	1425	0	1225	4	0
4	A	14	0	13	0	0
4	C	28	0	26	0	0
5	C	15	0	0	0	0
6	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2	0	0	0	0
All	All	3819	0	3331	17	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 2.

All (17) 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:100:MET:HG3	2:B:78:LEU:CD1	2.29	0.63
3:C:30:VAL:HG21	3:C:106:VAL:HG12	1.86	0.58
3:C:135:THR:HG23	3:C:171:THR:HG22	1.93	0.50
1:A:134:THR:HG22	1:A:136:LYS:H	1.76	0.50
1:A:49:LYS:HZ3	2:B:159:TYR:HA	1.76	0.50
2:B:127:VAL:O	2:B:216:GLY:HA3	2.13	0.48
1:A:54:TYR:CE2	1:A:141:VAL:HG21	2.50	0.46
2:B:40:PHE:CD2	2:B:71:PHE:HE2	2.32	0.46
2:B:78:LEU:HG	2:B:79:ARG:CG	2.48	0.44
3:C:189:ALA:HB1	3:C:194:TYR:CD2	2.54	0.43
1:A:30:ASP:OD1	1:A:32:THR:HG23	2.19	0.42
2:B:55:LEU:O	2:B:93:PHE:HA	2.19	0.42
1:A:67:VAL:HG12	1:A:147:LEU:HD21	2.02	0.42
1:A:43:TYR:HA	1:A:47:ILE:HB	2.01	0.41
1:A:45:SER:OG	2:B:213:TYR:CB	2.69	0.41
1:A:49:LYS:NZ	2:B:159:TYR:HA	2.36	0.41
3:C:32:ILE:HD11	3:C:99:ILE:CD1	2.52	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	123/163 (76%)	113 (92%)	10 (8%)	0	100	100
2	B	192/223 (86%)	184 (96%)	8 (4%)	0	100	100
3	C	187/230 (81%)	177 (95%)	10 (5%)	0	100	100
All	All	502/616 (82%)	474 (94%)	28 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	103/145 (71%)	100 (97%)	3 (3%)	48	79
2	B	120/198 (61%)	119 (99%)	1 (1%)	85	94
3	C	140/199 (70%)	135 (96%)	5 (4%)	40	75
All	All	363/542 (67%)	354 (98%)	9 (2%)	53	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	SER
1	A	142	SER
1	A	163	HIS
2	B	94	ILE
3	C	36	TYR
3	C	63	ASN
3	C	69	ASP
3	C	168	CYS
3	C	184	TRP

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	500	1	14,14,15	0.30	0	15,19,21	2.02	2 (13%)
5	SO4	C	301	-	4,4,4	0.30	0	6,6,6	0.08	0
5	SO4	C	302	-	4,4,4	0.40	0	6,6,6	0.30	0
5	SO4	C	303	-	4,4,4	0.22	0	6,6,6	0.26	0
4	NAG	C	304	3	14,14,15	0.26	0	15,19,21	1.03	1 (6%)
4	NAG	C	305	3	14,14,15	0.36	0	15,19,21	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	500	1	-	0/6/23/26	0/1/1/1
5	SO4	C	301	-	-	0/0/0/0	0/0/0/0
5	SO4	C	302	-	-	0/0/0/0	0/0/0/0
5	SO4	C	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	304	3	-	0/6/23/26	0/1/1/1
4	NAG	C	305	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	NAG	O5-C1-C2	-2.80	107.57	111.47
4	A	500	NAG	C1-C2-N2	2.34	114.49	110.49
4	A	500	NAG	C1-O5-C5	6.96	121.75	112.17

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

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	127/163 (77%)	0.02	1 (0%) 86 76	80, 108, 160, 174	0
2	B	194/223 (86%)	0.57	19 (9%) 8 7	110, 187, 242, 253	0
3	C	189/230 (82%)	0.14	10 (5%) 27 20	92, 143, 229, 245	0
All	All	510/616 (82%)	0.27	30 (5%) 23 17	80, 150, 233, 253	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	181	VAL	7.0
2	B	180	HIS	5.3
2	B	167	VAL	4.6
3	C	175	LEU	4.5
2	B	109	VAL	3.9
2	B	111	LEU	3.9
2	B	168	ALA	3.7
2	B	189	THR	3.5
2	B	172	ALA	3.1
2	B	147	LEU	3.0
2	B	182	SER	3.0
3	C	127	PHE	2.9
3	C	173	GLU	2.8
2	B	203	ILE	2.8
1	A	121	THR	2.8
2	B	188	THR	2.8
2	B	191	PRO	2.7
2	B	107	ILE	2.7
2	B	138	VAL	2.7
2	B	117	THR	2.6
3	C	183	PHE	2.6
2	B	225	SER	2.5
3	C	134	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	136	VAL	2.2
2	B	148	VAL	2.1
3	C	129	TRP	2.1
3	C	170	VAL	2.1
3	C	176	ASP	2.1
2	B	228	GLU	2.1
3	C	174	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q < 0.9
5	SO4	C	302	5/5	0.77	0.31	0.57	168,171,174,176	0
4	NAG	C	305	14/15	0.58	0.28	0.55	178,203,214,214	0
4	NAG	C	304	14/15	0.88	0.19	-0.23	197,208,219,221	0
4	NAG	A	500	14/15	0.93	0.22	-0.28	108,111,120,129	0
5	SO4	C	303	5/5	0.89	0.18	-0.93	176,179,181,181	0
5	SO4	C	301	5/5	0.87	0.20	-	178,183,185,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.