



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:05 am GMT

PDB ID : 4RSU  
Title : Crystal structure of the light and hvem complex  
Authors : Liu, W.; Ramagoal, U.A.; Himmel, D.; Bonanno, J.B.; Nathenson, S.G.; Almo, S.C.; Atoms-to-Animals: The Immune Function Network (IFN); New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2014-11-11  
Resolution : 2.30 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](mailto: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.

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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 : trunk28620  
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) : recalc28949

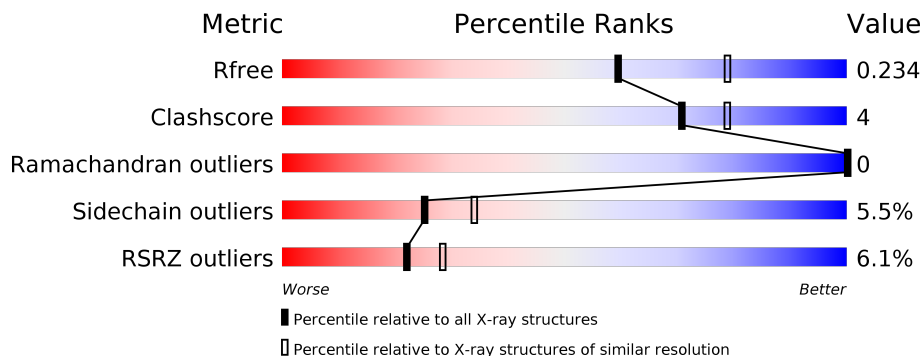
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 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	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 79%, yellow 79%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>79%</span> <span>10%</span> <span>10%</span> </div> </div>
1	B	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 75%, yellow 75%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>10%</span> <span>14%</span> </div> </div>
1	C	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, green 5%, green 72%, yellow 72%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>72%</span> <span>11%</span> <span>16%</span> </div> </div>
1	G	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 83%, yellow 83%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>5%</span> <span>9%</span> </div> </div>
1	H	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 78%, yellow 78%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>78%</span> <span>12%</span> <span>9%</span> </div> </div>
1	I	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, green 5%, green 75%, yellow 75%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>75%</span> <span>11%</span> <span>11%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	134	
2	E	134	
2	F	134	
2	J	134	
2	K	134	
2	L	134	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	301	-	-	-	X
3	CL	H	301	-	-	-	X
4	GOL	B	303	-	-	-	X
5	NAG	D	202	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11553 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 Tumor necrosis factor ligand superfamily member 14, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1140	727	199	211	3			
1	B	142	Total	C	N	O	S	0	0	0
			1093	697	189	204	3			
1	C	138	Total	C	N	O	S	0	0	0
			1069	684	185	197	3			
1	G	150	Total	C	N	O	S	0	0	0
			1149	732	200	214	3			
1	H	150	Total	C	N	O	S	0	0	0
			1149	732	200	214	3			
1	I	147	Total	C	N	O	S	0	0	0
			1125	716	197	209	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	HIS	-	EXPRESSION TAG	UNP O43557
A	77	HIS	-	EXPRESSION TAG	UNP O43557
A	78	HIS	-	EXPRESSION TAG	UNP O43557
A	79	HIS	-	EXPRESSION TAG	UNP O43557
A	80	HIS	-	EXPRESSION TAG	UNP O43557
A	81	HIS	-	EXPRESSION TAG	UNP O43557
A	82	GLY	-	EXPRESSION TAG	UNP O43557
A	214	GLU	LYS	CONFLICT	UNP O43557
B	76	HIS	-	EXPRESSION TAG	UNP O43557
B	77	HIS	-	EXPRESSION TAG	UNP O43557
B	78	HIS	-	EXPRESSION TAG	UNP O43557
B	79	HIS	-	EXPRESSION TAG	UNP O43557
B	80	HIS	-	EXPRESSION TAG	UNP O43557
B	81	HIS	-	EXPRESSION TAG	UNP O43557
B	82	GLY	-	EXPRESSION TAG	UNP O43557
B	214	GLU	LYS	CONFLICT	UNP O43557

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Chain	Residue	Modelled	Actual	Comment	Reference
C	76	HIS	-	EXPRESSION TAG	UNP O43557
C	77	HIS	-	EXPRESSION TAG	UNP O43557
C	78	HIS	-	EXPRESSION TAG	UNP O43557
C	79	HIS	-	EXPRESSION TAG	UNP O43557
C	80	HIS	-	EXPRESSION TAG	UNP O43557
C	81	HIS	-	EXPRESSION TAG	UNP O43557
C	82	GLY	-	EXPRESSION TAG	UNP O43557
C	214	GLU	LYS	CONFLICT	UNP O43557
G	76	HIS	-	EXPRESSION TAG	UNP O43557
G	77	HIS	-	EXPRESSION TAG	UNP O43557
G	78	HIS	-	EXPRESSION TAG	UNP O43557
G	79	HIS	-	EXPRESSION TAG	UNP O43557
G	80	HIS	-	EXPRESSION TAG	UNP O43557
G	81	HIS	-	EXPRESSION TAG	UNP O43557
G	82	GLY	-	EXPRESSION TAG	UNP O43557
G	214	GLU	LYS	CONFLICT	UNP O43557
H	76	HIS	-	EXPRESSION TAG	UNP O43557
H	77	HIS	-	EXPRESSION TAG	UNP O43557
H	78	HIS	-	EXPRESSION TAG	UNP O43557
H	79	HIS	-	EXPRESSION TAG	UNP O43557
H	80	HIS	-	EXPRESSION TAG	UNP O43557
H	81	HIS	-	EXPRESSION TAG	UNP O43557
H	82	GLY	-	EXPRESSION TAG	UNP O43557
H	214	GLU	LYS	CONFLICT	UNP O43557
I	76	HIS	-	EXPRESSION TAG	UNP O43557
I	77	HIS	-	EXPRESSION TAG	UNP O43557
I	78	HIS	-	EXPRESSION TAG	UNP O43557
I	79	HIS	-	EXPRESSION TAG	UNP O43557
I	80	HIS	-	EXPRESSION TAG	UNP O43557
I	81	HIS	-	EXPRESSION TAG	UNP O43557
I	82	GLY	-	EXPRESSION TAG	UNP O43557
I	214	GLU	LYS	CONFLICT	UNP O43557

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	105	Total	C	N	O	S	0	0	0
			761	458	136	149	18			
2	E	101	Total	C	N	O	S	0	0	0
			732	443	131	140	18			
2	F	98	Total	C	N	O	S	0	0	0
			705	425	126	136	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	106	Total	C	N	O	S	0	0	0
			766	461	137	150	18			
2	K	106	Total	C	N	O	S	0	0	0
			768	463	137	150	18			
2	L	104	Total	C	N	O	S	0	0	0
			741	445	133	145	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	37	ARG	-	EXPRESSION TAG	UNP Q92956
D	38	SER	-	EXPRESSION TAG	UNP Q92956
D	163	THR	-	EXPRESSION TAG	UNP Q92956
D	164	GLY	-	EXPRESSION TAG	UNP Q92956
D	165	HIS	-	EXPRESSION TAG	UNP Q92956
D	166	HIS	-	EXPRESSION TAG	UNP Q92956
D	167	HIS	-	EXPRESSION TAG	UNP Q92956
D	168	HIS	-	EXPRESSION TAG	UNP Q92956
D	169	HIS	-	EXPRESSION TAG	UNP Q92956
D	170	HIS	-	EXPRESSION TAG	UNP Q92956
E	37	ARG	-	EXPRESSION TAG	UNP Q92956
E	38	SER	-	EXPRESSION TAG	UNP Q92956
E	163	THR	-	EXPRESSION TAG	UNP Q92956
E	164	GLY	-	EXPRESSION TAG	UNP Q92956
E	165	HIS	-	EXPRESSION TAG	UNP Q92956
E	166	HIS	-	EXPRESSION TAG	UNP Q92956
E	167	HIS	-	EXPRESSION TAG	UNP Q92956
E	168	HIS	-	EXPRESSION TAG	UNP Q92956
E	169	HIS	-	EXPRESSION TAG	UNP Q92956
E	170	HIS	-	EXPRESSION TAG	UNP Q92956
F	37	ARG	-	EXPRESSION TAG	UNP Q92956
F	38	SER	-	EXPRESSION TAG	UNP Q92956
F	163	THR	-	EXPRESSION TAG	UNP Q92956
F	164	GLY	-	EXPRESSION TAG	UNP Q92956
F	165	HIS	-	EXPRESSION TAG	UNP Q92956
F	166	HIS	-	EXPRESSION TAG	UNP Q92956
F	167	HIS	-	EXPRESSION TAG	UNP Q92956
F	168	HIS	-	EXPRESSION TAG	UNP Q92956
F	169	HIS	-	EXPRESSION TAG	UNP Q92956
F	170	HIS	-	EXPRESSION TAG	UNP Q92956
J	37	ARG	-	EXPRESSION TAG	UNP Q92956
J	38	SER	-	EXPRESSION TAG	UNP Q92956

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Chain	Residue	Modelled	Actual	Comment	Reference
J	163	THR	-	EXPRESSION TAG	UNP Q92956
J	164	GLY	-	EXPRESSION TAG	UNP Q92956
J	165	HIS	-	EXPRESSION TAG	UNP Q92956
J	166	HIS	-	EXPRESSION TAG	UNP Q92956
J	167	HIS	-	EXPRESSION TAG	UNP Q92956
J	168	HIS	-	EXPRESSION TAG	UNP Q92956
J	169	HIS	-	EXPRESSION TAG	UNP Q92956
J	170	HIS	-	EXPRESSION TAG	UNP Q92956
K	37	ARG	-	EXPRESSION TAG	UNP Q92956
K	38	SER	-	EXPRESSION TAG	UNP Q92956
K	163	THR	-	EXPRESSION TAG	UNP Q92956
K	164	GLY	-	EXPRESSION TAG	UNP Q92956
K	165	HIS	-	EXPRESSION TAG	UNP Q92956
K	166	HIS	-	EXPRESSION TAG	UNP Q92956
K	167	HIS	-	EXPRESSION TAG	UNP Q92956
K	168	HIS	-	EXPRESSION TAG	UNP Q92956
K	169	HIS	-	EXPRESSION TAG	UNP Q92956
K	170	HIS	-	EXPRESSION TAG	UNP Q92956
L	37	ARG	-	EXPRESSION TAG	UNP Q92956
L	38	SER	-	EXPRESSION TAG	UNP Q92956
L	163	THR	-	EXPRESSION TAG	UNP Q92956
L	164	GLY	-	EXPRESSION TAG	UNP Q92956
L	165	HIS	-	EXPRESSION TAG	UNP Q92956
L	166	HIS	-	EXPRESSION TAG	UNP Q92956
L	167	HIS	-	EXPRESSION TAG	UNP Q92956
L	168	HIS	-	EXPRESSION TAG	UNP Q92956
L	169	HIS	-	EXPRESSION TAG	UNP Q92956
L	170	HIS	-	EXPRESSION TAG	UNP Q92956

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

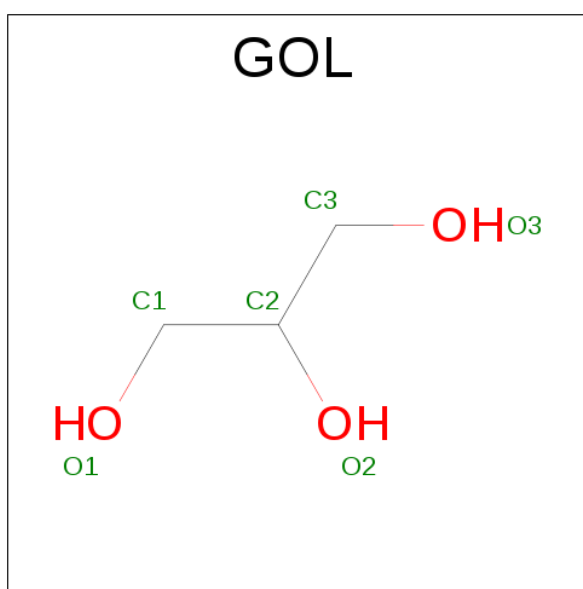
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Cl 3 3	0	0
3	K	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total 1	Cl 1	0	0
3	C	2	Total 2	Cl 2	0	0
3	A	2	Total 2	Cl 2	0	0
3	L	1	Total 1	Cl 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	I	1	Total 6	C 3	O 3	0	0

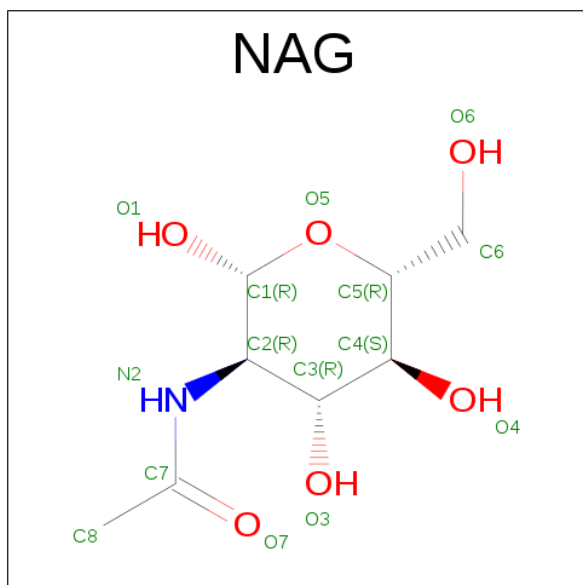
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	16	Total	O	0	0
			16	16		
6	C	12	Total	O	0	0
			12	12		

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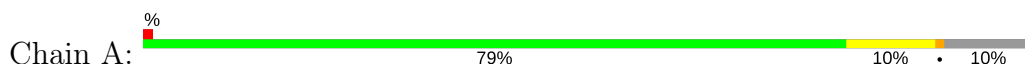
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	17	Total 17	O 17	0	0
6	E	4	Total 4	O 4	0	0
6	F	16	Total 16	O 16	0	0
6	G	47	Total 47	O 47	0	0
6	H	19	Total 19	O 19	0	0
6	I	21	Total 21	O 21	0	0
6	J	14	Total 14	O 14	0	0
6	K	4	Total 4	O 4	0	0
6	L	14	Total 14	O 14	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

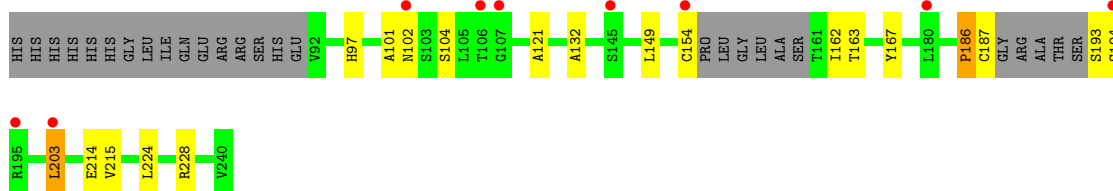
- Molecule 1: Tumor necrosis factor ligand superfamily member 14, soluble form



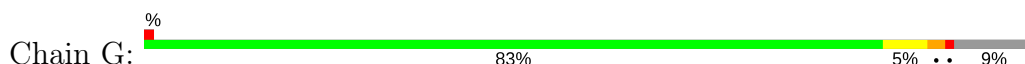
- Molecule 1: Tumor necrosis factor ligand superfamily member 14, soluble form



- Molecule 1: Tumor necrosis factor ligand superfamily member 14, soluble form



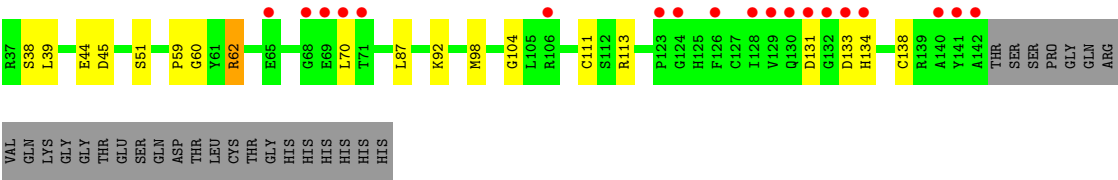
- Molecule 1: Tumor necrosis factor ligand superfamily member 14, soluble form



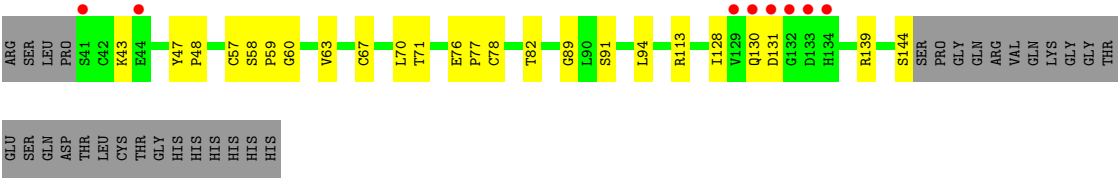
- Molecule 1: Tumor necrosis factor ligand superfamily member 14, soluble form



- Chain K: 



● Molecule 2: Tumor necrosis factor receptor superfamily member 14



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.65Å 113.60Å 163.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.30 35.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.92-2.30) 99.9 (35.03-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.188 , 0.231 0.194 , 0.234	Depositor DCC
$R_{free}$ test set	4631 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: GOL, NAG, CL

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	1.07	0/1167	1.05	8/1585 (0.5%)
1	B	0.98	0/1117	0.99	5/1514 (0.3%)
1	C	1.01	0/1093	0.97	1/1481 (0.1%)
1	G	1.11	0/1176	1.07	6/1597 (0.4%)
1	H	1.03	1/1176 (0.1%)	1.01	8/1597 (0.5%)
1	I	1.02	1/1151 (0.1%)	1.00	3/1562 (0.2%)
2	D	0.99	0/777	0.89	0/1052
2	E	0.88	1/747 (0.1%)	0.90	0/1010
2	F	0.96	0/718	0.97	1/970 (0.1%)
2	J	1.07	2/782 (0.3%)	1.03	1/1059 (0.1%)
2	K	0.92	0/784	0.99	3/1061 (0.3%)
2	L	1.02	1/755 (0.1%)	0.93	0/1022
All	All	1.01	6/11443 (0.1%)	0.99	36/15510 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	I	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	52	GLU	CD-OE1	7.15	1.33	1.25
2	J	52	GLU	CD-OE2	6.19	1.32	1.25
2	E	46	GLU	CD-OE1	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	198	TRP	CB-CG	-5.51	1.40	1.50
2	L	91	SER	CB-OG	-5.05	1.35	1.42

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	A	199	ASP	CB-CG-OD1	8.28	125.75	118.30
1	G	232	ARG	NE-CZ-NH1	-8.25	116.18	120.30
1	H	221	ASP	CB-CG-OD1	8.12	125.61	118.30
1	G	203	LEU	CA-CB-CG	7.20	131.85	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	191	THR	Peptide
1	C	186	PRO	Peptide
1	I	103	SER	Peptide

## 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	1140	0	1129	5	0
1	B	1093	0	1071	8	0
1	C	1069	0	1052	11	0
1	G	1149	0	1135	6	0
1	H	1149	0	1135	13	0
1	I	1125	0	1105	22	0
2	D	761	0	702	2	0
2	E	732	0	679	3	0
2	F	705	0	662	9	0
2	J	766	0	704	5	0
2	K	768	0	708	6	0
2	L	741	0	680	9	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	F	6	0	8	2	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
4	I	12	0	16	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0
5	L	14	0	13	0	0
6	A	39	0	0	0	0
6	B	16	0	0	0	0
6	C	12	0	0	0	0
6	D	17	0	0	0	0
6	E	4	0	0	0	0
6	F	16	0	0	3	0
6	G	47	0	0	2	0
6	H	19	0	0	0	0
6	I	21	0	0	0	0
6	J	14	0	0	0	0
6	K	4	0	0	0	0
6	L	14	0	0	0	0
All	All	11553	0	10891	92	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.

The worst 5 of 92 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:I:189:ARG:HB3	1:I:189:ARG:HH21	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:ALA:N	1:I:104:SER:OG	2.04	0.91
1:I:105:LEU:HD13	1:I:227:LEU:HD11	1.58	0.85
1:H:189:ARG:HD3	1:I:189:ARG:HG3	1.60	0.83
1:I:117:GLN:O	2:K:92:LYS:NZ	2.12	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	147/165 (89%)	144 (98%)	3 (2%)	0	100	100
1	B	136/165 (82%)	132 (97%)	4 (3%)	0	100	100
1	C	132/165 (80%)	126 (96%)	6 (4%)	0	100	100
1	G	148/165 (90%)	145 (98%)	3 (2%)	0	100	100
1	H	148/165 (90%)	143 (97%)	5 (3%)	0	100	100
1	I	143/165 (87%)	139 (97%)	4 (3%)	0	100	100
2	D	103/134 (77%)	102 (99%)	1 (1%)	0	100	100
2	E	97/134 (72%)	96 (99%)	1 (1%)	0	100	100
2	F	94/134 (70%)	93 (99%)	1 (1%)	0	100	100
2	J	104/134 (78%)	102 (98%)	2 (2%)	0	100	100
2	K	104/134 (78%)	101 (97%)	3 (3%)	0	100	100
2	L	102/134 (76%)	99 (97%)	3 (3%)	0	100	100
All	All	1458/1794 (81%)	1422 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	120/135 (89%)	115 (96%)	5 (4%)	34	47
1	B	116/135 (86%)	113 (97%)	3 (3%)	51	69
1	C	113/135 (84%)	108 (96%)	5 (4%)	33	45
1	G	121/135 (90%)	116 (96%)	5 (4%)	35	48
1	H	121/135 (90%)	117 (97%)	4 (3%)	43	59
1	I	118/135 (87%)	110 (93%)	8 (7%)	18	24
2	D	86/111 (78%)	83 (96%)	3 (4%)	41	56
2	E	83/111 (75%)	75 (90%)	8 (10%)	10	11
2	F	81/111 (73%)	76 (94%)	5 (6%)	21	28
2	J	86/111 (78%)	80 (93%)	6 (7%)	18	22
2	K	86/111 (78%)	78 (91%)	8 (9%)	10	12
2	L	82/111 (74%)	75 (92%)	7 (8%)	12	15
All	All	1213/1476 (82%)	1146 (94%)	67 (6%)	25	34

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	105	LEU
1	H	203	LEU
2	L	67	CYS
1	G	189	ARG
1	H	102	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	134	HIS
1	G	184	GLN
1	I	129	HIS
2	J	86	HIS

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Mol	Chain	Res	Type
2	K	134	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 for Mogul analysis.

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	GOL	B	303	-	5,5,5	0.44	0	5,5,5	0.40	0
4	GOL	C	302	-	5,5,5	0.41	0	5,5,5	0.72	0
4	GOL	D	201	-	5,5,5	0.42	0	5,5,5	0.78	0
5	NAG	D	202	2	14,14,15	1.29	1 (7%)	15,19,21	2.68	5 (33%)
5	NAG	E	202	2	14,14,15	0.94	1 (7%)	15,19,21	1.45	2 (13%)
4	GOL	F	201	-	5,5,5	0.22	0	5,5,5	1.34	0
4	GOL	G	303	-	5,5,5	0.27	0	5,5,5	0.80	0
4	GOL	H	302	-	5,5,5	0.91	0	5,5,5	0.38	0
4	GOL	I	302	-	5,5,5	0.49	0	5,5,5	1.12	1 (20%)
4	GOL	I	303	-	5,5,5	0.45	0	5,5,5	0.95	0
5	NAG	J	201	2	14,14,15	0.72	0	15,19,21	2.38	4 (26%)
5	NAG	K	202	2	14,14,15	0.77	1 (7%)	15,19,21	1.94	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	L	202	2	14,14,15	1.27	2 (14%)	15,19,21	1.83	3 (20%)

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	GOL	B	303	-	-	0/4/4/4	0/0/0/0
4	GOL	C	302	-	-	0/4/4/4	0/0/0/0
4	GOL	D	201	-	-	0/4/4/4	0/0/0/0
5	NAG	D	202	2	-	0/6/23/26	0/1/1/1
5	NAG	E	202	2	-	0/6/23/26	0/1/1/1
4	GOL	F	201	-	-	0/4/4/4	0/0/0/0
4	GOL	G	303	-	-	0/4/4/4	0/0/0/0
4	GOL	H	302	-	-	0/4/4/4	0/0/0/0
4	GOL	I	302	-	-	0/4/4/4	0/0/0/0
4	GOL	I	303	-	-	0/4/4/4	0/0/0/0
5	NAG	J	201	2	-	0/6/23/26	0/1/1/1
5	NAG	K	202	2	-	0/6/23/26	0/1/1/1
5	NAG	L	202	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	202	NAG	O5-C1	-3.15	1.38	1.43
5	K	202	NAG	C1-C2	2.13	1.55	1.52
5	E	202	NAG	C1-C2	2.81	1.56	1.52
5	L	202	NAG	C1-C2	3.02	1.56	1.52
5	D	202	NAG	C1-C2	4.05	1.58	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	202	NAG	O5-C1-C2	-4.89	104.67	111.47
5	L	202	NAG	C3-C4-C5	-3.22	104.55	110.22
5	D	202	NAG	O5-C1-C2	-2.94	107.39	111.47
5	J	201	NAG	C3-C4-C5	-2.84	105.21	110.22
5	D	202	NAG	O7-C7-C8	-2.46	117.57	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	201	GOL	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	149/165 (90%)	-0.25	1 (0%) 87 90	20, 27, 44, 82	0
1	B	142/165 (86%)	-0.21	1 (0%) 87 90	20, 31, 57, 91	0
1	C	138/165 (83%)	0.10	9 (6%) 20 26	20, 31, 62, 85	0
1	G	150/165 (90%)	-0.26	1 (0%) 87 90	18, 25, 45, 73	0
1	H	150/165 (90%)	-0.13	5 (3%) 47 54	20, 32, 58, 73	0
1	I	147/165 (89%)	0.08	8 (5%) 26 33	20, 31, 70, 89	0
2	D	105/134 (78%)	-0.30	4 (3%) 41 48	23, 33, 61, 90	0
2	E	101/134 (75%)	0.82	16 (15%) 2 3	33, 52, 91, 108	0
2	F	98/134 (73%)	0.08	10 (10%) 7 10	25, 38, 81, 100	0
2	J	106/134 (79%)	-0.00	10 (9%) 9 12	25, 36, 63, 91	0
2	K	106/134 (79%)	0.90	19 (17%) 2 2	32, 52, 88, 113	0
2	L	104/134 (77%)	0.04	8 (7%) 14 19	23, 36, 76, 137	0
All	All	1496/1794 (83%)	0.04	92 (6%) 22 28	18, 33, 73, 137	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	133	ASP	7.1
2	K	134	HIS	7.1
2	L	131	ASP	6.9
2	L	132	GLY	6.6
2	E	141	TYR	6.3

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	D	202	14/15	0.84	0.27	2.85	73,87,99,112	0
4	GOL	B	303	6/6	0.89	0.19	2.68	44,48,49,53	0
3	CL	B	301	1/1	0.99	0.13	2.55	31,31,31,31	0
3	CL	H	301	1/1	0.98	0.16	2.14	33,33,33,33	0
4	GOL	I	303	6/6	0.97	0.18	1.86	32,35,37,37	0
4	GOL	G	303	6/6	0.96	0.13	1.73	40,44,45,46	0
4	GOL	D	201	6/6	0.98	0.14	1.42	31,33,34,36	0
4	GOL	I	302	6/6	0.94	0.25	1.39	33,33,36,37	0
4	GOL	H	302	6/6	0.92	0.18	1.26	36,37,38,40	0
4	GOL	F	201	6/6	0.94	0.17	0.97	38,40,42,48	0
3	CL	I	301	1/1	0.98	0.17	0.61	37,37,37,37	0
3	CL	G	301	1/1	1.00	0.15	0.59	25,25,25,25	0
4	GOL	C	302	6/6	0.95	0.18	0.36	33,35,37,38	0
3	CL	B	302	1/1	0.97	0.10	0.15	48,48,48,48	0
3	CL	G	304	1/1	0.93	0.10	-0.02	43,43,43,43	0
3	CL	C	301	1/1	0.98	0.12	-0.10	40,40,40,40	0
3	CL	A	301	1/1	0.99	0.15	-0.13	29,29,29,29	0
3	CL	A	302	1/1	0.98	0.08	-1.18	37,37,37,37	0
3	CL	L	201	1/1	0.98	0.09	-1.57	46,46,46,46	0
3	CL	E	201	1/1	0.94	0.07	-1.91	45,45,45,45	0
3	CL	K	201	1/1	0.98	0.08	-1.97	46,46,46,46	0
3	CL	C	303	1/1	0.98	0.06	-5.23	42,42,42,42	0
5	NAG	L	202	14/15	0.84	0.26	-	64,78,86,87	0
5	NAG	K	202	14/15	0.83	0.28	-	71,82,93,93	0
5	NAG	J	201	14/15	0.83	0.23	-	54,70,85,88	0
5	NAG	E	202	14/15	0.83	0.21	-	74,84,93,94	0
3	CL	G	302	1/1	0.98	0.05	-	35,35,35,35	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.