Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 11:33 PM EDT

PDB ID	:	4G6J
Title	:	Crystal structure of human IL-1beta in complex with the therapeutic antibody binding fragment of canakinumab
Authors	:	Blech, M.; Hoerer, S.
Deposited on	:	2012-07-19
Resolution	:	2.03 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 (i) 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 (1)) were used in the production of this report:

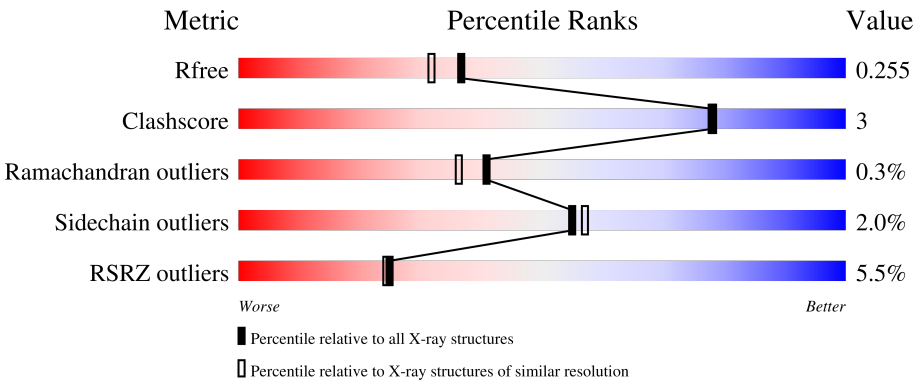
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	A	158	10%, 90%, • • 6%
2	H	218	5%, 91%, 9%
3	L	212	2%, 89%, 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4769 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-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	1193	757	197	231	8	21	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P01584
A	154	LEU	-	expression tag	UNP P01584
A	155	VAL	-	expression tag	UNP P01584
A	156	PRO	-	expression tag	UNP P01584
A	157	ARG	-	expression tag	UNP P01584

- Molecule 2 is a protein called heavy chain of antibody binding fragment of canakinumab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1644	1039	281	318	6	20	0	0

- Molecule 3 is a protein called light chain of antibody binding fragment of canakinumab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	1629	1022	272	331	4	18	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	65	65	65	0	0
4	H	122	122	122	0	0

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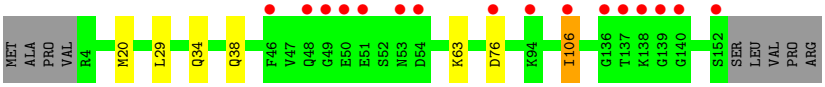
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	116	116	116	0	0

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.

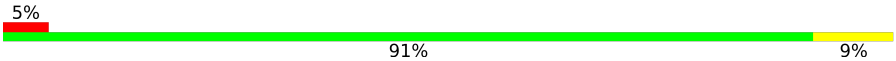
- Molecule 1: Interleukin-1 beta

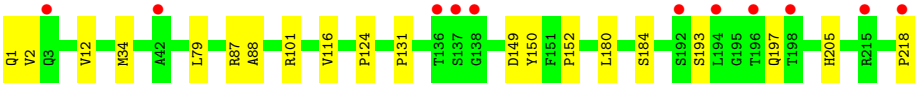
Chain A:



- Molecule 2: heavy chain of antibody binding fragment of canakinumab

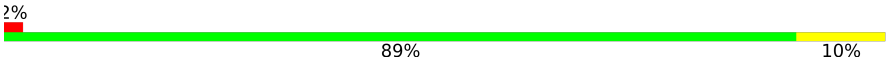
Chain H:





- Molecule 3: light chain of antibody binding fragment of canakinumab

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.06Å 37.30Å 189.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.03 74.52 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.36-2.03) 98.6 (74.52-2.03)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.226 , 0.252 0.225 , 0.255	Depositor DCC
R_{free} test set	1893 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4769	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	A	0.37	0/1215	0.63	0/1633
2	H	0.35	0/1685	0.64	0/2299
3	L	0.35	0/1666	0.60	0/2262
All	All	0.36	0/4566	0.63	0/6194

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	1193	0	1189	1	0
2	H	1644	0	1606	12	0
3	L	1629	0	1584	13	0
4	A	65	0	0	0	0
4	H	122	0	0	0	0
4	L	116	0	0	0	0
All	All	4769	0	4379	25	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 3.

All (25) 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)
3:L:106:ILE:H	3:L:166:GLN:HE22	1.27	0.81
2:H:1:GLN:HG3	2:H:2:VAL:H	1.57	0.69
2:H:12:VAL:HG13	2:H:116:VAL:HG12	1.77	0.66
3:L:22:THR:HG22	3:L:72:THR:HG22	1.80	0.63
1:A:38:GLN:HE22	2:H:101:ARG:H	1.50	0.58
2:H:152:PRO:O	2:H:205:HIS:HE1	1.90	0.54
3:L:108:ARG:HH12	3:L:111:ALA:HB2	1.73	0.53
2:H:87:ARG:O	2:H:116:VAL:HG21	2.09	0.52
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.93	0.51
2:H:1:GLN:HG3	2:H:2:VAL:N	2.26	0.50
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.96	0.48
2:H:131:PRO:HG2	2:H:218:PRO:HB3	1.97	0.47
3:L:21:ILE:HG21	3:L:102:THR:HG21	1.97	0.47
2:H:88:ALA:HA	2:H:116:VAL:HG23	1.97	0.46
2:H:149:ASP:HB3	2:H:180:LEU:HD13	1.96	0.46
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.97	0.45
3:L:106:ILE:N	3:L:166:GLN:HE22	2.07	0.44
3:L:18:LYS:HG3	3:L:76:ASN:HA	1.99	0.44
3:L:36:TYR:HE1	3:L:89:HIS:HB3	1.83	0.44
3:L:106:ILE:H	3:L:166:GLN:NE2	2.07	0.42
3:L:8:PRO:HG2	3:L:11:GLN:HB2	2.02	0.42
3:L:83:ALA:HB2	3:L:106:ILE:HG12	2.02	0.42
3:L:2:ILE:HG12	3:L:27:GLN:HB2	2.01	0.42
2:H:193:SER:OG	2:H:197:GLN:HB3	2.21	0.41
3:L:19:VAL:HG21	3:L:78:LEU:HD13	2.03	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	147/158 (93%)	140 (95%)	5 (3%)	2 (1%)	11 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
3	L	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
All	All	573/588 (97%)	552 (96%)	19 (3%)	2 (0%)	41	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	106	ILE

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	137/145 (94%)	132 (96%)	5 (4%)	35	32
2	H	181/181 (100%)	180 (99%)	1 (1%)	86	89
3	L	188/188 (100%)	184 (98%)	4 (2%)	53	55
All	All	506/514 (98%)	496 (98%)	10 (2%)	55	57

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	29	LEU
1	A	34	GLN
1	A	76	ASP
1	A	106	ILE
2	H	184	SER
3	L	14	THR
3	L	49	LYS
3	L	89	HIS
3	L	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
2	H	1	GLN
2	H	84	ASN
2	H	205	HIS
3	L	11	GLN
3	L	155	GLN
3	L	166	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	A	148/158 (93%)	0.75	16 (10%)	5	5	23, 42, 74, 94	2 (1%)
2	H	218/218 (100%)	0.27	11 (5%)	28	28	19, 29, 51, 58	4 (1%)
3	L	212/212 (100%)	0.27	5 (2%)	59	58	18, 32, 51, 76	5 (2%)
All	All	578/588 (98%)	0.39	32 (5%)	25	24	18, 33, 59, 94	11 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ASN	7.6
1	A	139	GLY	7.0
3	L	212	GLY	6.7
2	H	215	ARG	5.7
1	A	106	ILE	5.0
1	A	136	GLY	4.6
1	A	49	GLY	4.2
1	A	140	GLY	4.1
2	H	138	GLY	3.9
1	A	152	SER	3.9
1	A	51	GLU	3.8
3	L	126	LYS	3.3
2	H	42	ALA	3.1
2	H	198	THR	3.1
3	L	24	ARG	2.9
2	H	218	PRO	2.6
2	H	136	THR	2.6
1	A	138	LYS	2.5
1	A	137	THR	2.5
1	A	50	GLU	2.4
1	A	48	GLN	2.4
1	A	46	PHE	2.4
2	H	196	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	194	LEU	2.3
1	A	94	LYS	2.2
2	H	192	SER	2.2
1	A	54	ASP	2.1
3	L	202	SER	2.0
2	H	137	SER	2.0
3	L	76	ASN	2.0
1	A	76	ASP	2.0
2	H	3	GLN	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 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.