wwPDB X-ray Structure Validation Summary Report (i)

Feb 11, 2024 – 11:09 PM EST

PDB ID	:	3DKB
Title	:	Crystal Structure of A20, 2.5 angstrom
Authors	:	Lin, S.-C.; Chung, J.Y.; Lo, Y.-C.; Wu, H.
Deposited on	:	2008-06-24
Resolution	:	2.50 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*
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 (i)) were used in the production of this report:

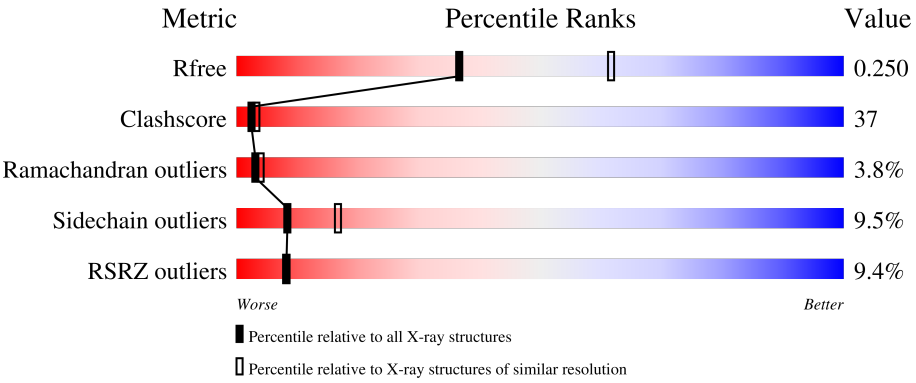
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	390	7% 33% 49% 8% 10%
1	B	390	8% 39% 42% 8% 10%
1	C	390	11% 33% 50% 7% 10%
1	D	390	8% 35% 49% 6% 10%
1	E	390	9% 39% 44% 7% 10%

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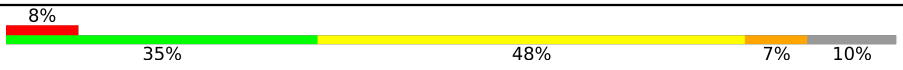
Mol	Chain	Length	Quality of chain
1	F	390	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17550 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, alpha-induced protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	B	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	C	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	D	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	E	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	F	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5981	MET	-	expression tag	UNP P21580
A	5982	GLY	-	expression tag	UNP P21580
A	5983	SER	-	expression tag	UNP P21580
A	5984	SER	-	expression tag	UNP P21580
A	5985	HIS	-	expression tag	UNP P21580
A	5986	HIS	-	expression tag	UNP P21580
A	5987	HIS	-	expression tag	UNP P21580
A	5988	HIS	-	expression tag	UNP P21580
A	5989	HIS	-	expression tag	UNP P21580
A	5990	HIS	-	expression tag	UNP P21580
A	5991	SER	-	expression tag	UNP P21580
A	5992	SER	-	expression tag	UNP P21580
A	5993	GLY	-	expression tag	UNP P21580
A	5994	LEU	-	expression tag	UNP P21580
A	5995	VAL	-	expression tag	UNP P21580
A	5996	PRO	-	expression tag	UNP P21580
A	5997	ARG	-	expression tag	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5998	GLY	-	expression tag	UNP P21580
A	5999	SER	-	expression tag	UNP P21580
A	6000	HIS	-	expression tag	UNP P21580
B	981	MET	-	expression tag	UNP P21580
B	982	GLY	-	expression tag	UNP P21580
B	983	SER	-	expression tag	UNP P21580
B	984	SER	-	expression tag	UNP P21580
B	985	HIS	-	expression tag	UNP P21580
B	986	HIS	-	expression tag	UNP P21580
B	987	HIS	-	expression tag	UNP P21580
B	988	HIS	-	expression tag	UNP P21580
B	989	HIS	-	expression tag	UNP P21580
B	990	HIS	-	expression tag	UNP P21580
B	991	SER	-	expression tag	UNP P21580
B	992	SER	-	expression tag	UNP P21580
B	993	GLY	-	expression tag	UNP P21580
B	994	LEU	-	expression tag	UNP P21580
B	995	VAL	-	expression tag	UNP P21580
B	996	PRO	-	expression tag	UNP P21580
B	997	ARG	-	expression tag	UNP P21580
B	998	GLY	-	expression tag	UNP P21580
B	999	SER	-	expression tag	UNP P21580
B	1000	HIS	-	expression tag	UNP P21580
C	1981	MET	-	expression tag	UNP P21580
C	1982	GLY	-	expression tag	UNP P21580
C	1983	SER	-	expression tag	UNP P21580
C	1984	SER	-	expression tag	UNP P21580
C	1985	HIS	-	expression tag	UNP P21580
C	1986	HIS	-	expression tag	UNP P21580
C	1987	HIS	-	expression tag	UNP P21580
C	1988	HIS	-	expression tag	UNP P21580
C	1989	HIS	-	expression tag	UNP P21580
C	1990	HIS	-	expression tag	UNP P21580
C	1991	SER	-	expression tag	UNP P21580
C	1992	SER	-	expression tag	UNP P21580
C	1993	GLY	-	expression tag	UNP P21580
C	1994	LEU	-	expression tag	UNP P21580
C	1995	VAL	-	expression tag	UNP P21580
C	1996	PRO	-	expression tag	UNP P21580
C	1997	ARG	-	expression tag	UNP P21580
C	1998	GLY	-	expression tag	UNP P21580
C	1999	SER	-	expression tag	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2000	HIS	-	expression tag	UNP P21580
D	2981	MET	-	expression tag	UNP P21580
D	2982	GLY	-	expression tag	UNP P21580
D	2983	SER	-	expression tag	UNP P21580
D	2984	SER	-	expression tag	UNP P21580
D	2985	HIS	-	expression tag	UNP P21580
D	2986	HIS	-	expression tag	UNP P21580
D	2987	HIS	-	expression tag	UNP P21580
D	2988	HIS	-	expression tag	UNP P21580
D	2989	HIS	-	expression tag	UNP P21580
D	2990	HIS	-	expression tag	UNP P21580
D	2991	SER	-	expression tag	UNP P21580
D	2992	SER	-	expression tag	UNP P21580
D	2993	GLY	-	expression tag	UNP P21580
D	2994	LEU	-	expression tag	UNP P21580
D	2995	VAL	-	expression tag	UNP P21580
D	2996	PRO	-	expression tag	UNP P21580
D	2997	ARG	-	expression tag	UNP P21580
D	2998	GLY	-	expression tag	UNP P21580
D	2999	SER	-	expression tag	UNP P21580
D	3000	HIS	-	expression tag	UNP P21580
E	3981	MET	-	expression tag	UNP P21580
E	3982	GLY	-	expression tag	UNP P21580
E	3983	SER	-	expression tag	UNP P21580
E	3984	SER	-	expression tag	UNP P21580
E	3985	HIS	-	expression tag	UNP P21580
E	3986	HIS	-	expression tag	UNP P21580
E	3987	HIS	-	expression tag	UNP P21580
E	3988	HIS	-	expression tag	UNP P21580
E	3989	HIS	-	expression tag	UNP P21580
E	3990	HIS	-	expression tag	UNP P21580
E	3991	SER	-	expression tag	UNP P21580
E	3992	SER	-	expression tag	UNP P21580
E	3993	GLY	-	expression tag	UNP P21580
E	3994	LEU	-	expression tag	UNP P21580
E	3995	VAL	-	expression tag	UNP P21580
E	3996	PRO	-	expression tag	UNP P21580
E	3997	ARG	-	expression tag	UNP P21580
E	3998	GLY	-	expression tag	UNP P21580
E	3999	SER	-	expression tag	UNP P21580
E	4000	HIS	-	expression tag	UNP P21580
F	4981	MET	-	expression tag	UNP P21580

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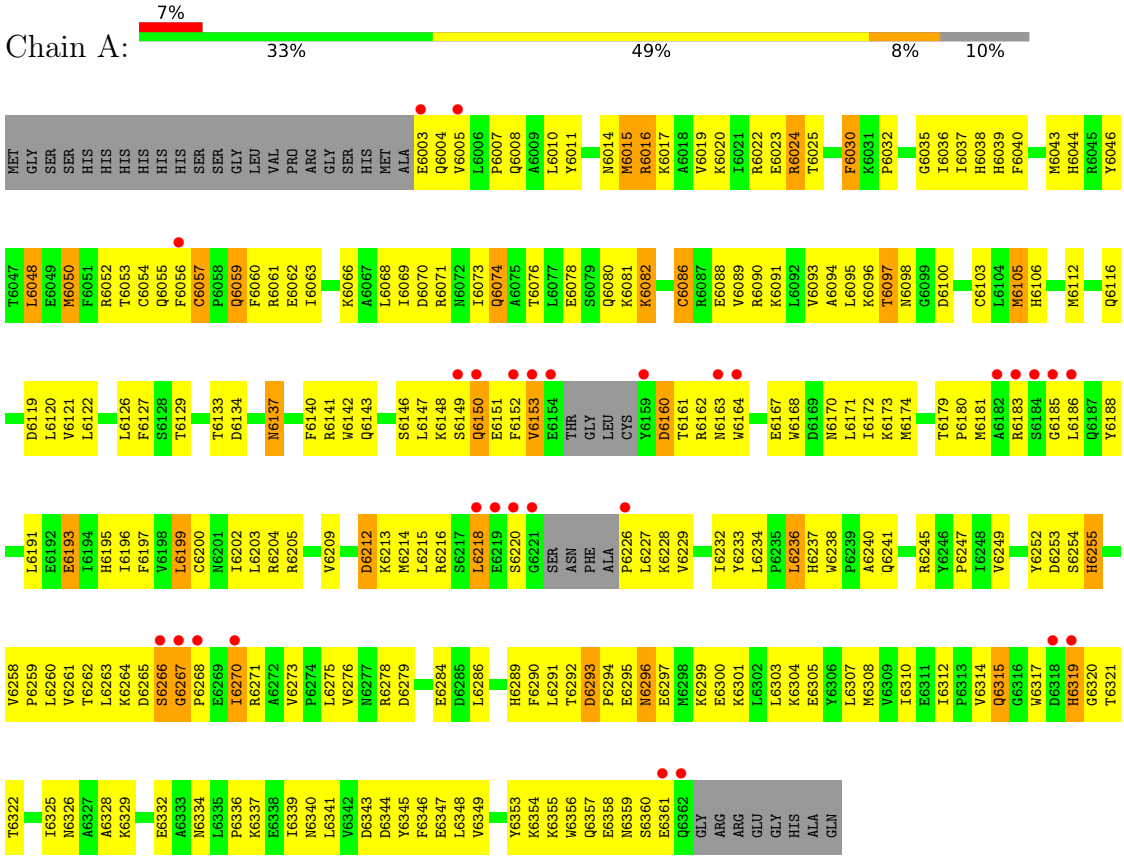
Chain	Residue	Modelled	Actual	Comment	Reference
F	4982	GLY	-	expression tag	UNP P21580
F	4983	SER	-	expression tag	UNP P21580
F	4984	SER	-	expression tag	UNP P21580
F	4985	HIS	-	expression tag	UNP P21580
F	4986	HIS	-	expression tag	UNP P21580
F	4987	HIS	-	expression tag	UNP P21580
F	4988	HIS	-	expression tag	UNP P21580
F	4989	HIS	-	expression tag	UNP P21580
F	4990	HIS	-	expression tag	UNP P21580
F	4991	SER	-	expression tag	UNP P21580
F	4992	SER	-	expression tag	UNP P21580
F	4993	GLY	-	expression tag	UNP P21580
F	4994	LEU	-	expression tag	UNP P21580
F	4995	VAL	-	expression tag	UNP P21580
F	4996	PRO	-	expression tag	UNP P21580
F	4997	ARG	-	expression tag	UNP P21580
F	4998	GLY	-	expression tag	UNP P21580
F	4999	SER	-	expression tag	UNP P21580
F	5000	HIS	-	expression tag	UNP P21580

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.

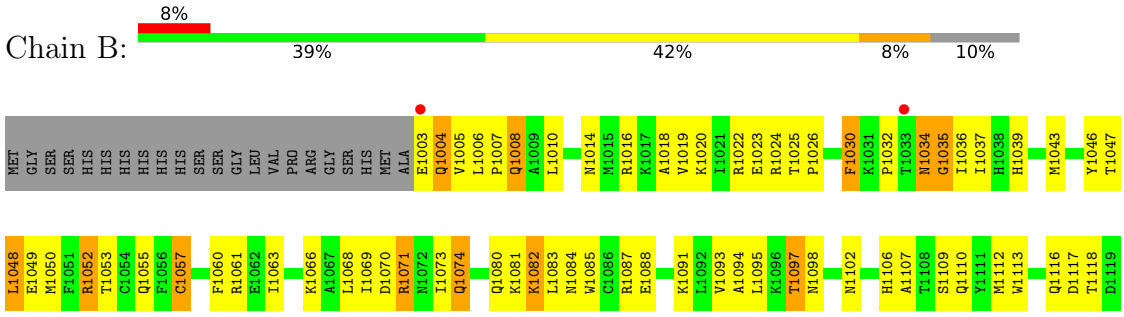
• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

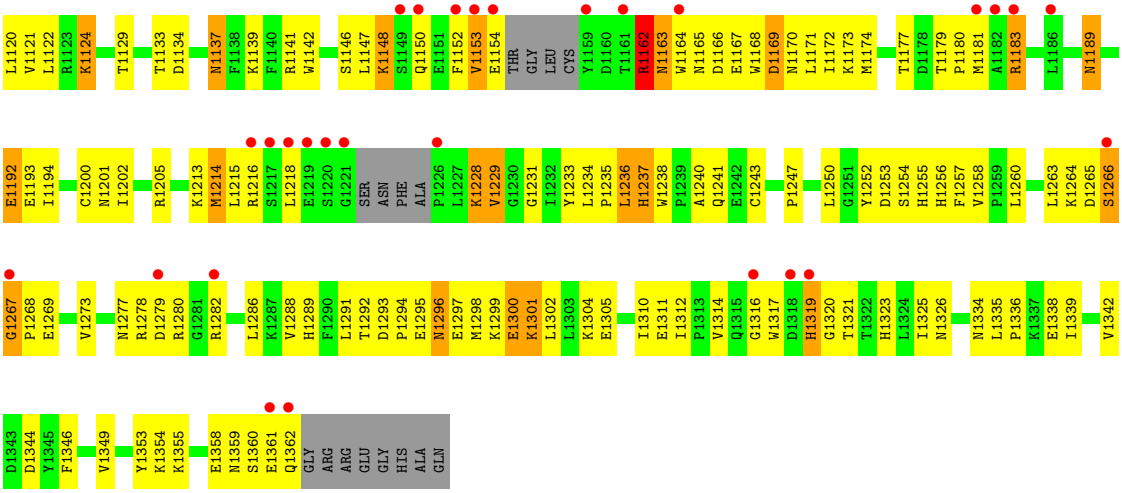
Chain A:



• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

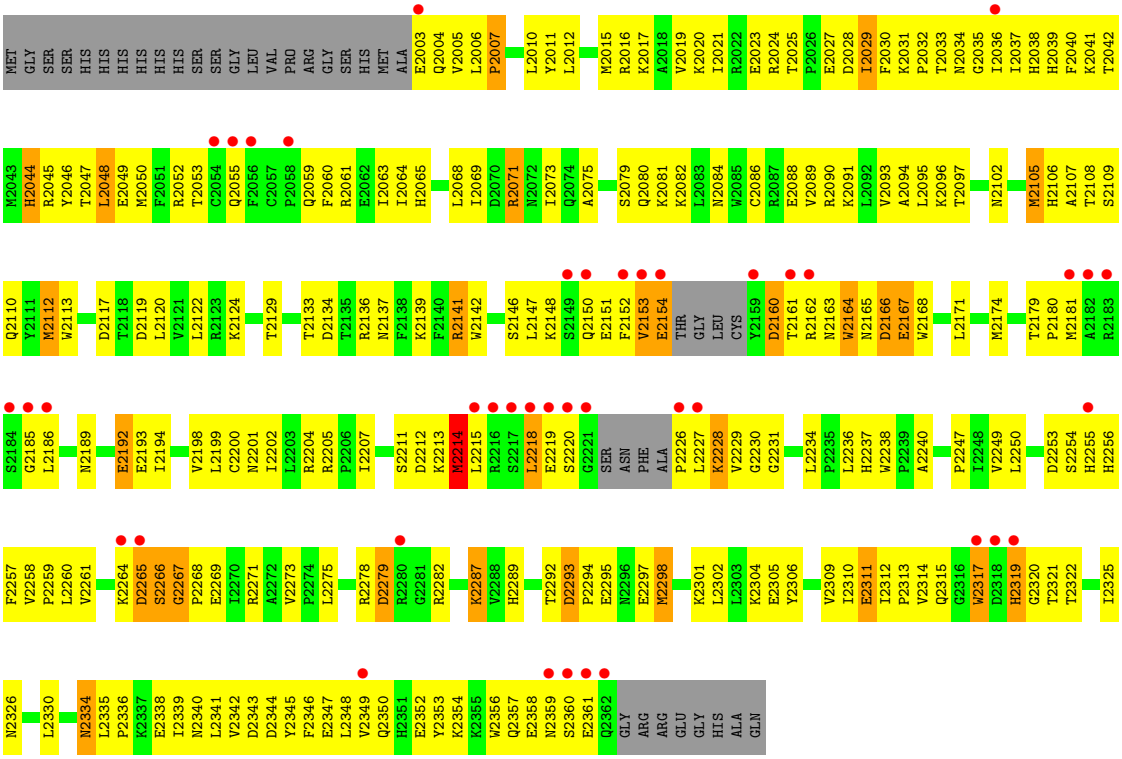
Chain B:





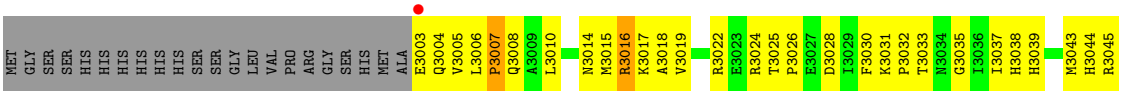
• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

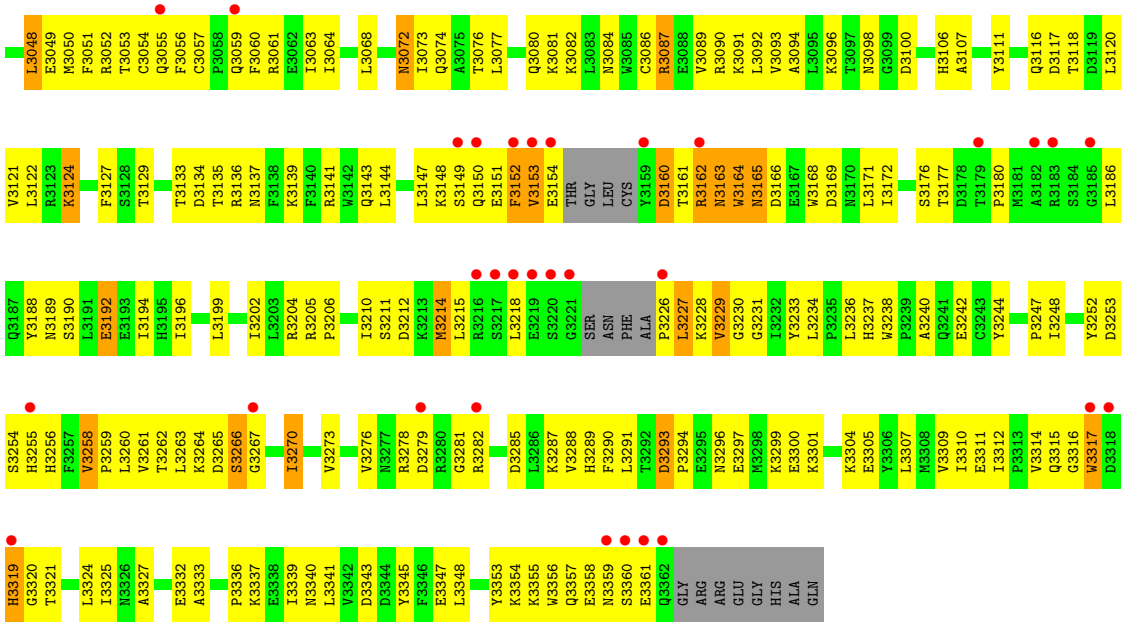
Chain C:



• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

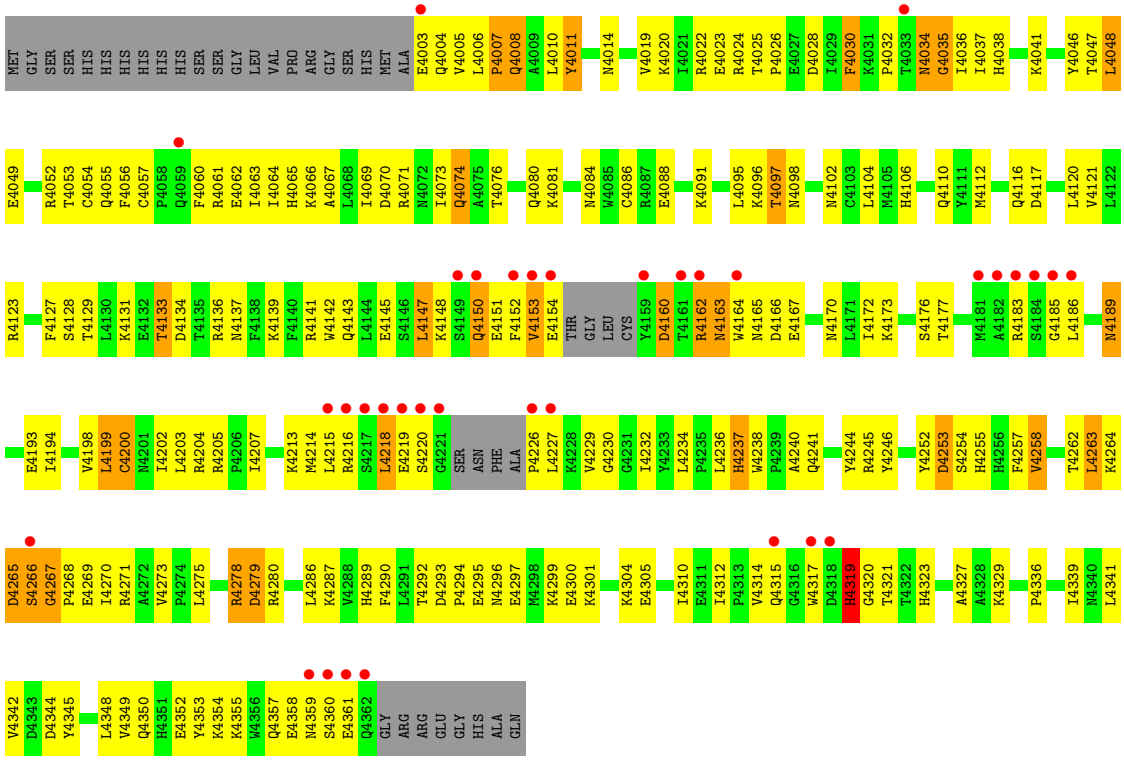
Chain D:





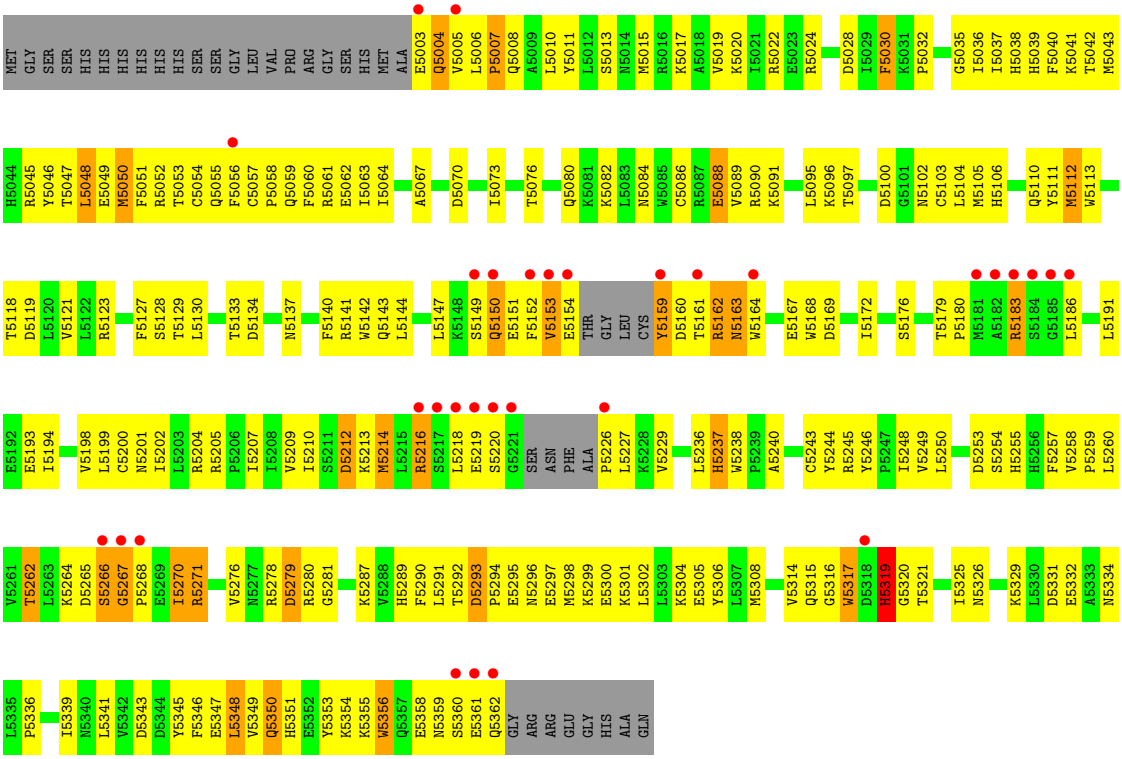
• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

Chain E:



• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

Chain F:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA E5003 Q5004 V5005 L5006 P5007 Q5008 A5009 L5010 Y5011 L5012 S5013 N5014 M5015 R5016 K5017 A5018 V5019 K5020 I5021 R5022 E5023 R5024 D5028 I5029 F5030 K5031 P5032 G5035 I5036 I5037 H5038 H5039 F5040 K5041 T5042 M5043
H5044 R5045 Y5046 T5047 L5048 E5049 M5050 F5051 R5052 T5053 C5054 Q5055 F5056 C5057 P5058 Q5059 F5060 R5061 E5062 I5063 I5064 A5067 D5070 I5073 T5076 Q5080 K5081 K5082 L5083 N5084 W5085 C5086 R5087 E5088 V5089 R5090 K5091 L5095 K5096 T5097 D5100 G5101 N5102 C5103 L5104 M5105 H5106 Q5110 Y5111 M5112 W5113
T5118 D5119 L5120 V5121 L5122 R5123 F5127 S5128 T5129 L5130 T5133 D5134 N5137 F5140 R5141 W5142 Q5143 L5144 L5147 K5148 S5149 Q5150 E5151 F5152 V5153 E5154 THR GLY LEU CYS Y5159 D5160 T5161 R5162 N5163 W5164 E5167 W5168 D5169 I5172 S5176 T5179 P5180 M5181 A5182 R5183 S5184 G5185 L5186 L5191
E5192 E5193 I5194 V5198 L5199 C5200 N5201 I5202 L5203 R5204 R5205 P5206 I5207 I5208 V5209 I5210 S5211 D5212 K5213 M5214 L5215 R5216 S5217 L5218 E5219 S5220 G5221 SER ASN PHE ALA P5226 L5227 K5228 V5229 L5236 H5237 W5238 P5239 A5240 C5243 Y5244 R5245 Y5246 P5247 I5248 V5249 L5250 D5253 S5254 H5255 H5256 F5257 V5258 P5259 L5260
V5261 T5262 L5263 K5264 D5265 S5266 G5267 P5268 E5269 I5270 R5271 V5276 N5277 R5278 D5279 R5280 G5281 K5287 V5288 H5289 F5290 L5291 T5292 D5293 P5294 E5295 N5296 E5297 M5298 K5299 E5300 K5301 L5302 L5303 K5304 E5305 Y5306 L5307 M5308 V5314 Q5315 G5316 W5317 D5318 N5319 G5320 T5321 I5325 N5326 K5329 L5330 D5331 E5332 A5333 N5334
L5335 P5336 I5339 N5340 L5341 V5342 D5343 D5344 Y5345 F5346 E5347 L5348 V5349 Q5350 H5351 E5352 Y5353 K5354 K5355 W5356 Q5357 E5358 N5359 S5360 E5361 Q5362 GLY ARG ARG GLU GLY HIS ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	123.64Å 123.64Å 143.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 29.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (25.00-2.50) 95.8 (29.74-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.246 0.207 , 0.250	Depositor DCC
R_{free} test set	8218 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.039 for h,-h-k,-l 0.488 for -k,-h,-l	Xtriage
Reported twinning fraction	0.476 for h+k,-k,-l	Depositor
Outliers	0 of 84471 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17550	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5482e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.43	0/2993	0.65	0/4045
1	B	0.47	0/2993	0.69	1/4045 (0.0%)
1	C	0.40	0/2993	0.65	0/4045
1	D	0.44	0/2993	0.66	0/4045
1	E	0.48	0/2993	0.68	0/4045
1	F	0.42	0/2993	0.66	1/4045 (0.0%)
All	All	0.44	0/17958	0.67	2/24270 (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	F	5348	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	1264	LYS	N-CA-C	5.12	124.83	111.00

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	2925	0	2915	216	0
1	B	2925	0	2915	208	0
1	C	2925	0	2915	227	0
1	D	2925	0	2915	230	0
1	E	2925	0	2915	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2925	0	2915	245	0
All	All	17550	0	17490	1309	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 37.

The worst 5 of 1309 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:6336:PRO:HD2	1:A:6339:ILE:HD11	1.19	1.17
1:B:1228:LYS:H	1:B:1228:LYS:HD2	1.14	1.11
1:C:2105:MET:HG3	1:C:2122:LEU:HB3	1.29	1.09
1:B:1189:ASN:ND2	1:B:1189:ASN:H	1.43	1.09
1:F:5336:PRO:HD2	1:F:5339:ILE:HD11	1.38	1.06

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	346/390 (89%)	297 (86%)	36 (10%)	13 (4%)	3	4
1	B	346/390 (89%)	298 (86%)	33 (10%)	15 (4%)	2	3
1	C	346/390 (89%)	294 (85%)	39 (11%)	13 (4%)	3	4
1	D	346/390 (89%)	298 (86%)	34 (10%)	14 (4%)	3	3
1	E	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	3	4
1	F	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	3	4
All	All	2076/2340 (89%)	1779 (86%)	218 (10%)	79 (4%)	3	4

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6004	GLN
1	A	6266	SER
1	A	6279	ASP
1	B	1004	GLN
1	B	1163	ASN

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	325/354 (92%)	291 (90%)	34 (10%)	7 13
1	B	325/354 (92%)	289 (89%)	36 (11%)	6 11
1	C	325/354 (92%)	296 (91%)	29 (9%)	9 19
1	D	325/354 (92%)	300 (92%)	25 (8%)	13 25
1	E	325/354 (92%)	294 (90%)	31 (10%)	8 17
1	F	325/354 (92%)	294 (90%)	31 (10%)	8 17
All	All	1950/2124 (92%)	1764 (90%)	186 (10%)	8 17

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3229	VAL
1	E	4200	CYS
1	D	3282	ARG
1	E	4062	GLU
1	E	4263	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	4004	GLN
1	F	5039	HIS
1	E	4044	HIS
1	E	4256	HIS

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Mol	Chain	Res	Type
1	F	5143	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	352/390 (90%)	0.32	29 (8%) 11 11	20, 62, 150, 195	0
1	B	352/390 (90%)	0.21	30 (8%) 10 10	19, 50, 142, 179	0
1	C	352/390 (90%)	0.52	41 (11%) 4 4	30, 66, 148, 185	0
1	D	352/390 (90%)	0.29	32 (9%) 9 9	23, 59, 145, 188	0
1	E	352/390 (90%)	0.24	35 (9%) 7 7	19, 52, 145, 175	0
1	F	352/390 (90%)	0.40	31 (8%) 10 10	28, 67, 146, 194	0
All	All	2112/2340 (90%)	0.33	198 (9%) 8 8	19, 59, 146, 195	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5153	VAL	22.8
1	C	2318	ASP	19.4
1	E	4153	VAL	18.3
1	D	3153	VAL	16.5
1	A	6150	GLN	15.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.