wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 03:24 pm BST

PDB ID	:	3MOP
Title	:	The ternary Death Domain complex of MyD88, IRAK4, and IRAK2
Authors	:	Lin, S.-C.; Lo, Y.-C.; Wu, H.
Deposited on	:	2010-04-23
Resolution	:	3.40 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 following versions of software and data (see references (1)) were used in the production of this report:

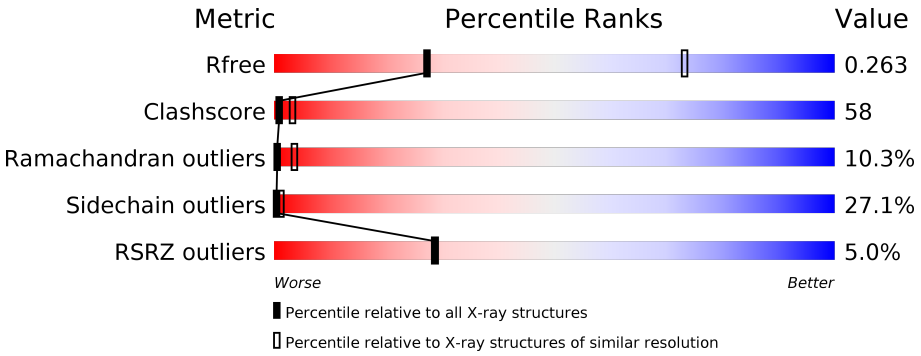
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 >=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	110	22% 31% 51% 13% • 5%
1	B	110	3% 30% 48% 16% • 5%
1	C	110	2% 25% 45% 25% • 5%
1	D	110	26% 47% 21% • 5%
1	E	110	19% 48% 25% • 5%
1	F	110	25% 48% 21% • 5%

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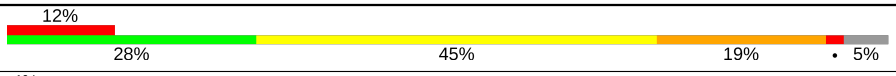
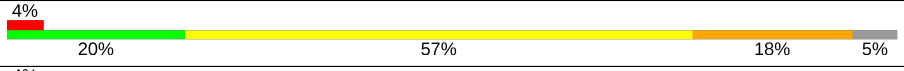
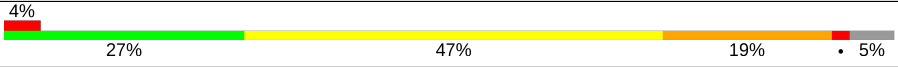
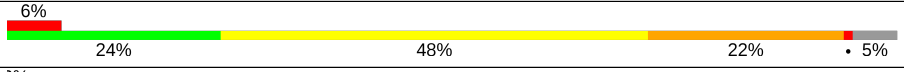
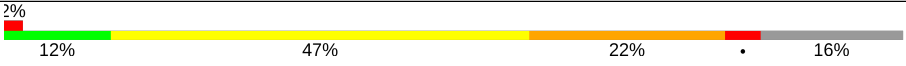
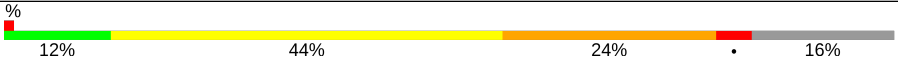
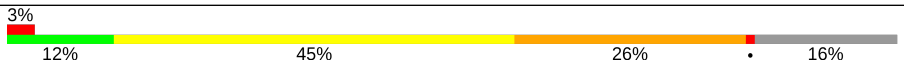
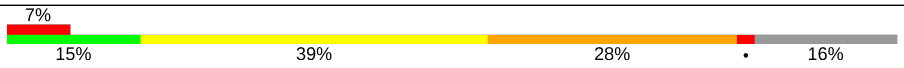
Mol	Chain	Length	Quality of chain
2	G	113	
2	H	113	
2	I	113	
2	J	113	
3	K	111	
3	L	111	
3	M	111	
3	N	111	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11534 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 Myeloid differentiation primary response protein MyD88.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			833	525	148	156	4			
1	B	105	Total	C	N	O	S	0	0	0
			833	525	148	156	4			
1	C	105	Total	C	N	O	S	0	0	0
			833	525	148	156	4			
1	D	105	Total	C	N	O	S	0	0	0
			833	525	148	156	4			
1	E	105	Total	C	N	O	S	0	0	0
			833	525	148	156	4			
1	F	105	Total	C	N	O	S	0	0	0
			833	525	148	156	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP Q99836
A	118	ALA	-	EXPRESSION TAG	UNP Q99836
A	119	ALA	-	EXPRESSION TAG	UNP Q99836
A	120	ALA	-	EXPRESSION TAG	UNP Q99836
A	121	LEU	-	EXPRESSION TAG	UNP Q99836
A	122	GLU	-	EXPRESSION TAG	UNP Q99836
A	123	HIS	-	EXPRESSION TAG	UNP Q99836
A	124	HIS	-	EXPRESSION TAG	UNP Q99836
A	125	HIS	-	EXPRESSION TAG	UNP Q99836
A	126	HIS	-	EXPRESSION TAG	UNP Q99836
A	127	HIS	-	EXPRESSION TAG	UNP Q99836
A	128	HIS	-	EXPRESSION TAG	UNP Q99836
B	19	MET	-	EXPRESSION TAG	UNP Q99836
B	118	ALA	-	EXPRESSION TAG	UNP Q99836
B	119	ALA	-	EXPRESSION TAG	UNP Q99836
B	120	ALA	-	EXPRESSION TAG	UNP Q99836
B	121	LEU	-	EXPRESSION TAG	UNP Q99836

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Chain	Residue	Modelled	Actual	Comment	Reference
B	122	GLU	-	EXPRESSION TAG	UNP Q99836
B	123	HIS	-	EXPRESSION TAG	UNP Q99836
B	124	HIS	-	EXPRESSION TAG	UNP Q99836
B	125	HIS	-	EXPRESSION TAG	UNP Q99836
B	126	HIS	-	EXPRESSION TAG	UNP Q99836
B	127	HIS	-	EXPRESSION TAG	UNP Q99836
B	128	HIS	-	EXPRESSION TAG	UNP Q99836
C	19	MET	-	EXPRESSION TAG	UNP Q99836
C	118	ALA	-	EXPRESSION TAG	UNP Q99836
C	119	ALA	-	EXPRESSION TAG	UNP Q99836
C	120	ALA	-	EXPRESSION TAG	UNP Q99836
C	121	LEU	-	EXPRESSION TAG	UNP Q99836
C	122	GLU	-	EXPRESSION TAG	UNP Q99836
C	123	HIS	-	EXPRESSION TAG	UNP Q99836
C	124	HIS	-	EXPRESSION TAG	UNP Q99836
C	125	HIS	-	EXPRESSION TAG	UNP Q99836
C	126	HIS	-	EXPRESSION TAG	UNP Q99836
C	127	HIS	-	EXPRESSION TAG	UNP Q99836
C	128	HIS	-	EXPRESSION TAG	UNP Q99836
D	19	MET	-	EXPRESSION TAG	UNP Q99836
D	118	ALA	-	EXPRESSION TAG	UNP Q99836
D	119	ALA	-	EXPRESSION TAG	UNP Q99836
D	120	ALA	-	EXPRESSION TAG	UNP Q99836
D	121	LEU	-	EXPRESSION TAG	UNP Q99836
D	122	GLU	-	EXPRESSION TAG	UNP Q99836
D	123	HIS	-	EXPRESSION TAG	UNP Q99836
D	124	HIS	-	EXPRESSION TAG	UNP Q99836
D	125	HIS	-	EXPRESSION TAG	UNP Q99836
D	126	HIS	-	EXPRESSION TAG	UNP Q99836
D	127	HIS	-	EXPRESSION TAG	UNP Q99836
D	128	HIS	-	EXPRESSION TAG	UNP Q99836
E	19	MET	-	EXPRESSION TAG	UNP Q99836
E	118	ALA	-	EXPRESSION TAG	UNP Q99836
E	119	ALA	-	EXPRESSION TAG	UNP Q99836
E	120	ALA	-	EXPRESSION TAG	UNP Q99836
E	121	LEU	-	EXPRESSION TAG	UNP Q99836
E	122	GLU	-	EXPRESSION TAG	UNP Q99836
E	123	HIS	-	EXPRESSION TAG	UNP Q99836
E	124	HIS	-	EXPRESSION TAG	UNP Q99836
E	125	HIS	-	EXPRESSION TAG	UNP Q99836
E	126	HIS	-	EXPRESSION TAG	UNP Q99836
E	127	HIS	-	EXPRESSION TAG	UNP Q99836

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Chain	Residue	Modelled	Actual	Comment	Reference
E	128	HIS	-	EXPRESSION TAG	UNP Q99836
F	19	MET	-	EXPRESSION TAG	UNP Q99836
F	118	ALA	-	EXPRESSION TAG	UNP Q99836
F	119	ALA	-	EXPRESSION TAG	UNP Q99836
F	120	ALA	-	EXPRESSION TAG	UNP Q99836
F	121	LEU	-	EXPRESSION TAG	UNP Q99836
F	122	GLU	-	EXPRESSION TAG	UNP Q99836
F	123	HIS	-	EXPRESSION TAG	UNP Q99836
F	124	HIS	-	EXPRESSION TAG	UNP Q99836
F	125	HIS	-	EXPRESSION TAG	UNP Q99836
F	126	HIS	-	EXPRESSION TAG	UNP Q99836
F	127	HIS	-	EXPRESSION TAG	UNP Q99836
F	128	HIS	-	EXPRESSION TAG	UNP Q99836

- Molecule 2 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	107	Total	C	N	O	S	0	0	0
			843	544	140	156	3			
2	H	107	Total	C	N	O	S	0	0	0
			843	544	140	156	3			
2	I	107	Total	C	N	O	S	0	0	0
			843	544	140	156	3			
2	J	107	Total	C	N	O	S	0	0	0
			843	544	140	156	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	MET	-	EXPRESSION TAG	UNP Q9NWZ3
G	3	GLY	-	EXPRESSION TAG	UNP Q9NWZ3
G	107	LEU	-	EXPRESSION TAG	UNP Q9NWZ3
G	108	GLU	-	EXPRESSION TAG	UNP Q9NWZ3
G	109	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
G	110	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
G	111	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
G	112	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
G	113	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
G	114	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
H	2	MET	-	EXPRESSION TAG	UNP Q9NWZ3
H	3	GLY	-	EXPRESSION TAG	UNP Q9NWZ3
H	107	LEU	-	EXPRESSION TAG	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	108	GLU	-	EXPRESSION TAG	UNP Q9NWZ3
H	109	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
H	110	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
H	111	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
H	112	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
H	113	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
H	114	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
I	2	MET	-	EXPRESSION TAG	UNP Q9NWZ3
I	3	GLY	-	EXPRESSION TAG	UNP Q9NWZ3
I	107	LEU	-	EXPRESSION TAG	UNP Q9NWZ3
I	108	GLU	-	EXPRESSION TAG	UNP Q9NWZ3
I	109	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
I	110	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
I	111	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
I	112	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
I	113	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
I	114	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
J	2	MET	-	EXPRESSION TAG	UNP Q9NWZ3
J	3	GLY	-	EXPRESSION TAG	UNP Q9NWZ3
J	107	LEU	-	EXPRESSION TAG	UNP Q9NWZ3
J	108	GLU	-	EXPRESSION TAG	UNP Q9NWZ3
J	109	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
J	110	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
J	111	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
J	112	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
J	113	HIS	-	EXPRESSION TAG	UNP Q9NWZ3
J	114	HIS	-	EXPRESSION TAG	UNP Q9NWZ3

- Molecule 3 is a protein called Interleukin-1 receptor-associated kinase-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	93	Total	C	N	O	S	0	0	0
			791	516	131	137	7			
3	L	93	Total	C	N	O	S	0	0	0
			791	516	131	137	7			
3	M	93	Total	C	N	O	S	0	0	0
			791	516	131	137	7			
3	N	93	Total	C	N	O	S	0	0	0
			791	516	131	137	7			

There are 4 discrepancies between the modelled and reference sequences:

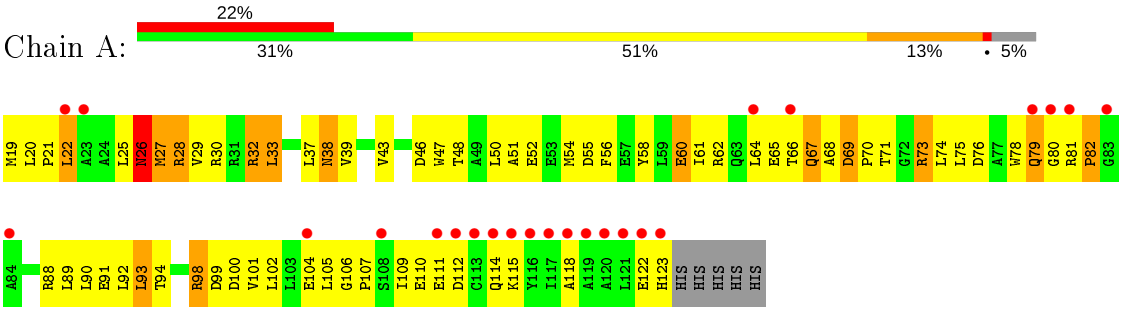
Chain	Residue	Modelled	Actual	Comment	Reference
K	50	TRP	ARG	ENGINEERED MUTATION	UNP O43187
L	50	TRP	ARG	ENGINEERED MUTATION	UNP O43187
M	50	TRP	ARG	ENGINEERED MUTATION	UNP O43187
N	50	TRP	ARG	ENGINEERED MUTATION	UNP O43187

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 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.

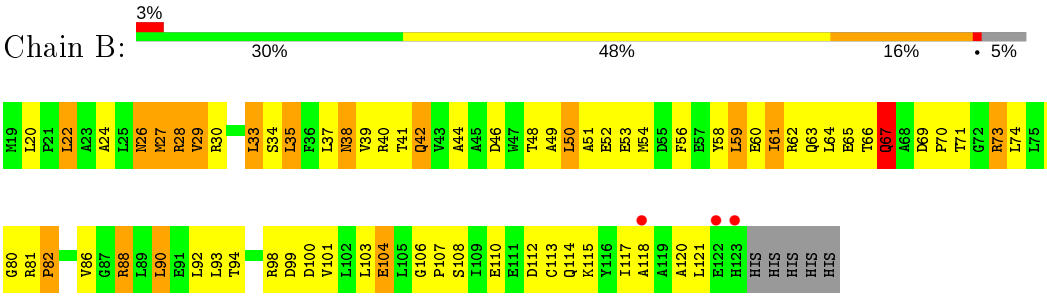
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain A:



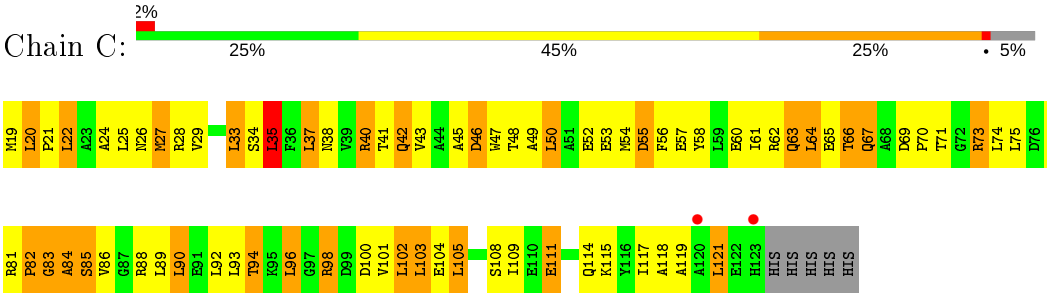
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain B:



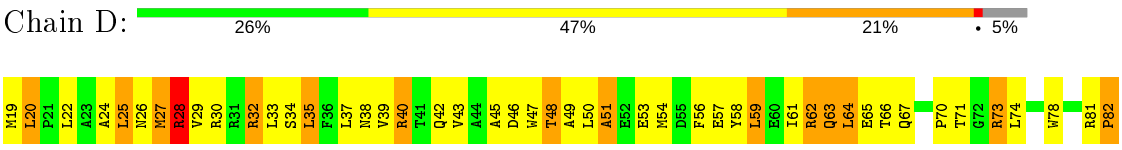
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain C:



- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain D:

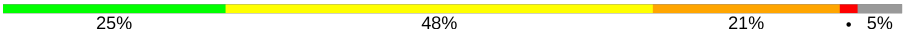


• Molecule 1: Myeloid differentiation primary response protein MyD88

Chain E:

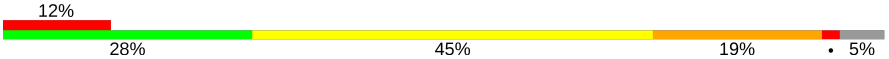
• Molecule 1: Myeloid differentiation primary response protein MyD88

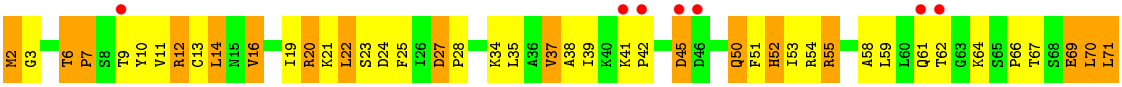
Chain F:

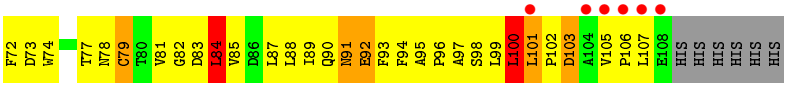


• Molecule 2: Interleukin-1 receptor-associated kinase 4

Chain G:

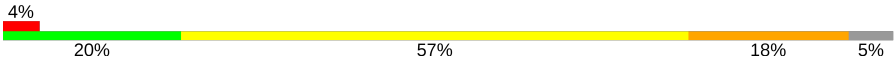


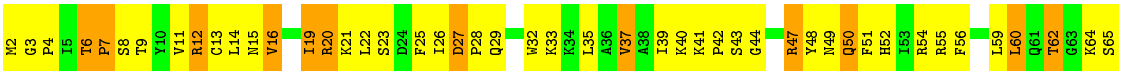


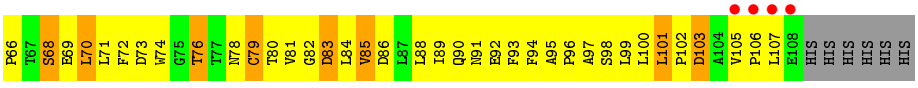


• Molecule 2: Interleukin-1 receptor-associated kinase 4

Chain H:

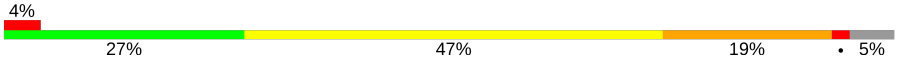


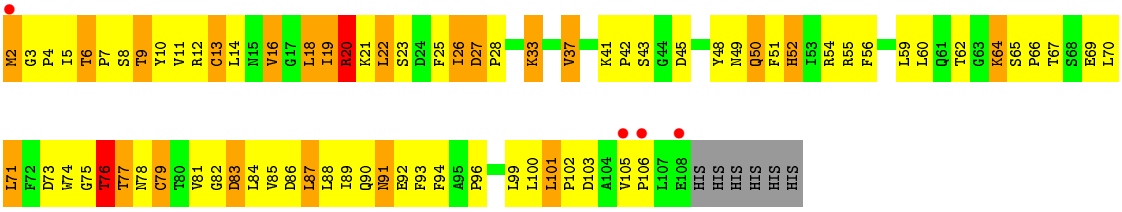




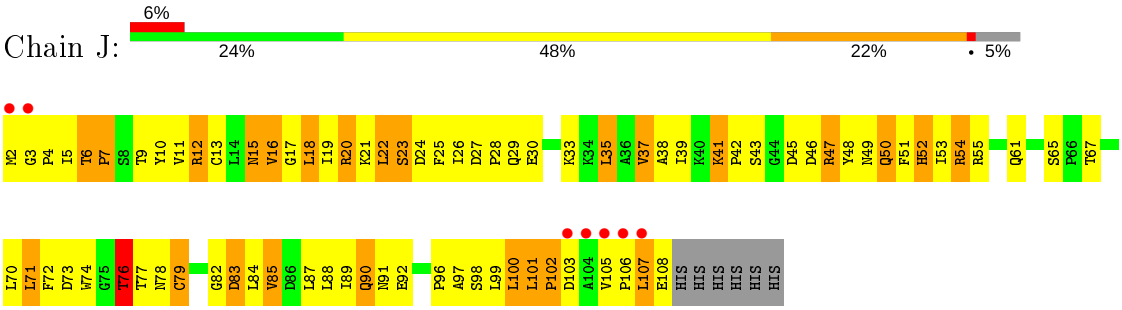
• Molecule 2: Interleukin-1 receptor-associated kinase 4

Chain I:

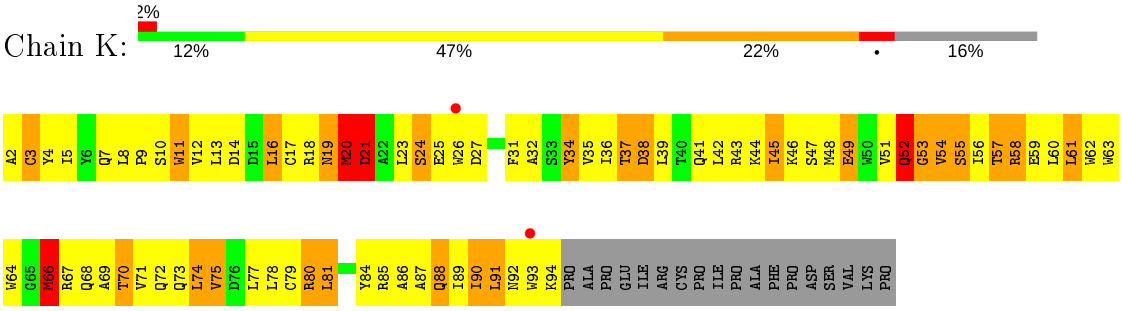




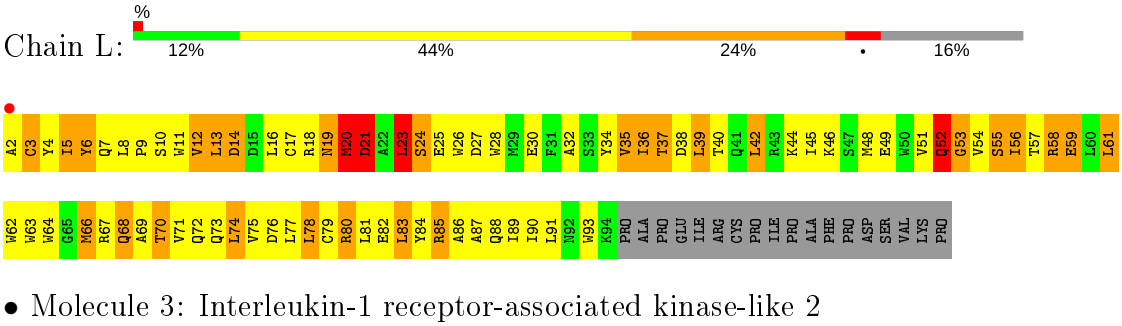
• Molecule 2: Interleukin-1 receptor-associated kinase 4



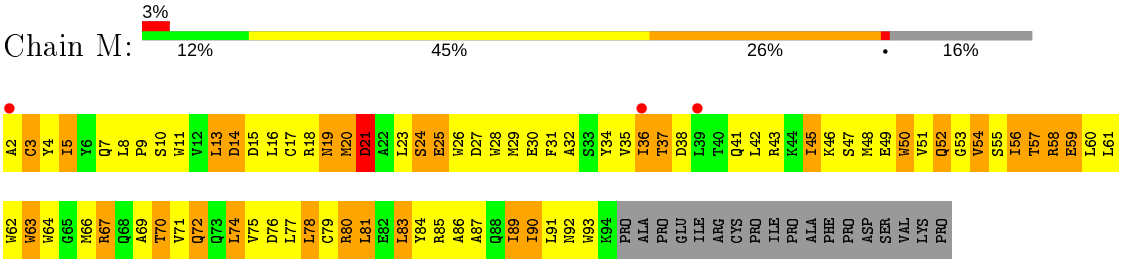
• Molecule 3: Interleukin-1 receptor-associated kinase-like 2



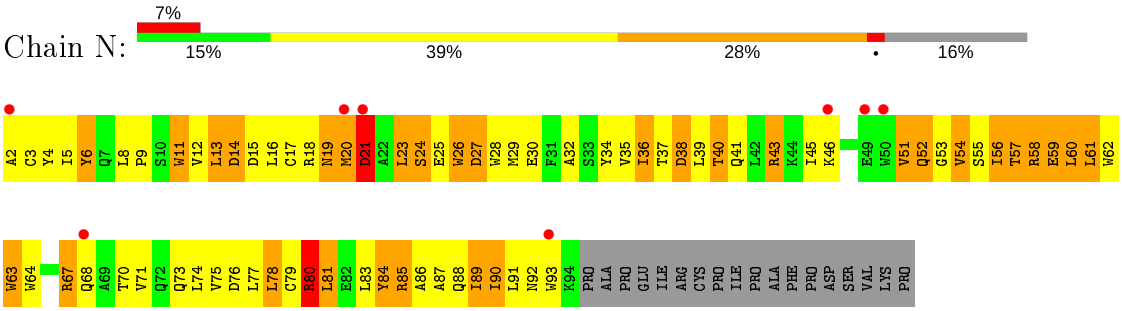
• Molecule 3: Interleukin-1 receptor-associated kinase-like 2



• Molecule 3: Interleukin-1 receptor-associated kinase-like 2



• Molecule 3: Interleukin-1 receptor-associated kinase-like 2


Chain N:
7%
15%
39%
28%
16%
A2 C3 Y4 I5 Y6 Q7 L8 P9 S10 W11 V12 L13 D14 D15 L16 C17 R18 N19 M20 D21 A22 L23 S24 E25 W26 D27 W28 M29 E30 F31 A32 S33 Y34 V35 I36 T37 D38 L39 T40 Q41 L42 R43 K44 I45 K46 E49 W50 V51 Q52 G53 V54 S55 I56 T57 R58 E59 L60 L61 W62
W63 W64 R67 Q68 A69 T70 V71 Q72 Q73 L74 V75 D76 L77 L78 C79 R80 L81 E82 L83 Y84 R85 A86 A87 Q88 I89 I90 L91 N92 W93 K94 PRO ALA PRO GLU ILE ARG CYS PRO ILE PRO ALA PHE PRO ASP SER VAL LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.71Å 307.12Å 187.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.40 30.26 – 3.34	Depositor EDS
% Data completeness (in resolution range)	82.3 (19.96-3.40) 79.6 (30.26-3.34)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.49 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.216 , 0.261 0.214 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	110.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 134.3	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	0.94	EDS
Total number of atoms	11534	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

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	0.42	0/845	0.63	0/1144
1	B	0.59	0/845	0.81	1/1144 (0.1%)
1	C	0.52	0/845	0.78	1/1144 (0.1%)
1	D	0.60	0/845	0.89	0/1144
1	E	0.70	0/845	1.00	5/1144 (0.4%)
1	F	0.55	0/845	0.81	0/1144
2	G	0.59	0/863	0.81	2/1174 (0.2%)
2	H	0.64	0/863	0.81	0/1174
2	I	0.59	0/863	0.78	1/1174 (0.1%)
2	J	0.47	0/863	0.69	0/1174
3	K	0.50	0/812	0.67	0/1106
3	L	0.56	0/812	0.77	2/1106 (0.2%)
3	M	0.50	0/812	0.66	0/1106
3	N	0.49	0/812	0.66	0/1106
All	All	0.56	0/11770	0.78	12/15984 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	23	LEU	CA-CB-CG	7.67	132.94	115.30
1	B	59	LEU	CA-CB-CG	-6.16	101.12	115.30
3	L	39	LEU	CA-CB-CG	5.89	128.84	115.30
1	E	121	LEU	CA-CB-CG	5.67	128.34	115.30
1	C	96	LEU	CA-CB-CG	5.57	128.12	115.30

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	833	0	844	86	0
1	B	833	0	844	88	0
1	C	833	0	844	106	0
1	D	833	0	844	110	0
1	E	833	0	844	119	0
1	F	833	0	844	113	0
2	G	843	0	849	100	0
2	H	843	0	849	116	0
2	I	843	0	849	102	0
2	J	843	0	849	107	0
3	K	791	0	784	101	0
3	L	791	0	784	117	0
3	M	791	0	784	103	0
3	N	791	0	784	107	0
All	All	11534	0	11596	1335	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 58.

The worst 5 of 1335 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:N:13:LEU:HD21	3:N:61:LEU:HD23	1.24	1.16
1:B:114:GLN:HA	1:B:117:ILE:HG22	1.23	1.12
3:L:20:MET:HB3	3:L:57:THR:HG21	1.29	1.11
2:G:100:LEU:HD22	2:G:101:LEU:HD22	1.22	1.10
2:H:2:MET:HG3	2:H:3:GLY:H	1.09	1.10

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	103/110 (94%)	74 (72%)	21 (20%)	8 (8%)	1 6
1	B	103/110 (94%)	75 (73%)	22 (21%)	6 (6%)	1 11
1	C	103/110 (94%)	65 (63%)	30 (29%)	8 (8%)	1 6
1	D	103/110 (94%)	70 (68%)	18 (18%)	15 (15%)	0 1
1	E	103/110 (94%)	68 (66%)	22 (21%)	13 (13%)	0 2
1	F	103/110 (94%)	65 (63%)	30 (29%)	8 (8%)	1 6
2	G	105/113 (93%)	77 (73%)	19 (18%)	9 (9%)	1 5
2	H	105/113 (93%)	80 (76%)	17 (16%)	8 (8%)	1 6
2	I	105/113 (93%)	76 (72%)	20 (19%)	9 (9%)	1 5
2	J	105/113 (93%)	77 (73%)	17 (16%)	11 (10%)	0 3
3	K	91/111 (82%)	64 (70%)	13 (14%)	14 (15%)	0 0
3	L	91/111 (82%)	61 (67%)	16 (18%)	14 (15%)	0 0
3	M	91/111 (82%)	64 (70%)	16 (18%)	11 (12%)	0 2
3	N	91/111 (82%)	63 (69%)	18 (20%)	10 (11%)	0 3
All	All	1402/1556 (90%)	979 (70%)	279 (20%)	144 (10%)	0 3

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	27	MET
1	C	82	PRO
1	C	84	ALA
1	D	28	ARG
1	D	65	GLU

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	87/92 (95%)	73 (84%)	14 (16%)	2 10
1	B	87/92 (95%)	67 (77%)	20 (23%)	1 2
1	C	87/92 (95%)	62 (71%)	25 (29%)	0 1
1	D	87/92 (95%)	68 (78%)	19 (22%)	1 3
1	E	87/92 (95%)	63 (72%)	24 (28%)	0 1
1	F	87/92 (95%)	61 (70%)	26 (30%)	0 1
2	G	94/100 (94%)	72 (77%)	22 (23%)	1 2
2	H	94/100 (94%)	75 (80%)	19 (20%)	1 3
2	I	94/100 (94%)	68 (72%)	26 (28%)	0 1
2	J	94/100 (94%)	66 (70%)	28 (30%)	0 1
3	K	85/101 (84%)	57 (67%)	28 (33%)	0 1
3	L	85/101 (84%)	58 (68%)	27 (32%)	0 1
3	M	85/101 (84%)	58 (68%)	27 (32%)	0 1
3	N	85/101 (84%)	55 (65%)	30 (35%)	0 1
All	All	1238/1356 (91%)	903 (73%)	335 (27%)	0 1

5 of 335 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	12	ARG
2	I	71	LEU
3	N	21	ASP
2	H	19	ILE
2	I	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	61	GLN

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Mol	Chain	Res	Type
2	I	61	GLN
3	N	7	GLN
2	G	90	GLN
2	H	91	ASN

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

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	105/110 (95%)	1.07	24 (22%) 0 1	120, 221, 385, 434	105 (100%)
1	B	105/110 (95%)	-0.45	3 (2%) 51 50	80, 138, 223, 329	0
1	C	105/110 (95%)	-0.41	2 (1%) 66 65	100, 163, 234, 335	0
1	D	105/110 (95%)	-0.63	0 100 100	87, 134, 192, 309	0
1	E	105/110 (95%)	-0.70	0 100 100	69, 119, 182, 292	0
1	F	105/110 (95%)	-0.49	0 100 100	85, 162, 254, 320	0
2	G	107/113 (94%)	0.24	13 (12%) 4 5	106, 183, 297, 329	0
2	H	107/113 (94%)	-0.36	4 (3%) 41 40	83, 141, 227, 297	0
2	I	107/113 (94%)	-0.29	4 (3%) 41 40	91, 145, 253, 307	0
2	J	107/113 (94%)	0.04	7 (6%) 18 20	115, 184, 274, 332	0
3	K	93/111 (83%)	-0.15	2 (2%) 62 60	121, 199, 285, 322	0
3	L	93/111 (83%)	-0.45	1 (1%) 80 79	116, 191, 261, 320	0
3	M	93/111 (83%)	-0.01	3 (3%) 47 46	126, 218, 286, 317	0
3	N	93/111 (83%)	0.21	8 (8%) 10 12	152, 227, 283, 304	0
All	All	1430/1556 (91%)	-0.17	71 (4%) 28 29	69, 171, 287, 434	105 (7%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	108	GLU	10.8
1	A	120	ALA	8.8
1	A	119	ALA	8.8
1	A	118	ALA	7.2
1	B	123	HIS	6.9

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.