wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 02:24 AM EST

PDB ID	:	3OQ9
Title	:	Structure of the FAS/FADD death domain assembly
Authors	:	Kabaleeswaran, V.; Wu, H.
Deposited on	:	2010-09-02
Resolution	:	6.80 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 (1)) were used in the production of this report:

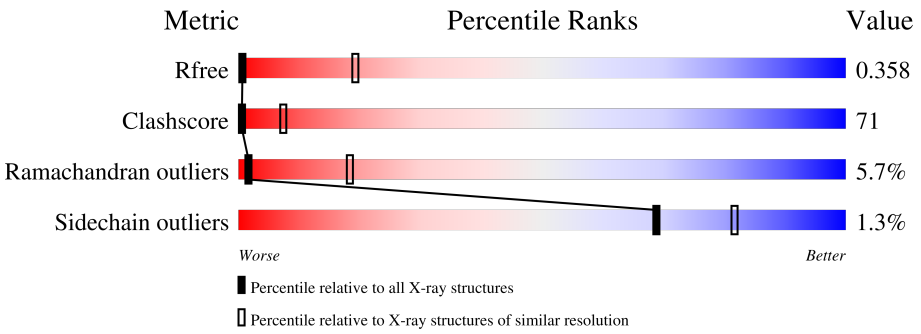
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 6.80 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	1003 (9.70-3.90)
Clashscore	141614	1067 (9.70-3.90)
Ramachandran outliers	138981	1001 (9.70-3.90)
Sidechain outliers	138945	1001 (9.70-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	86	29% 64% 7%
1	B	86	23% 69% 8%
1	C	86	26% 66% 8%
1	D	86	27% 65% 8%
1	E	86	26% 66% 8%
2	H	100	39% 52% • 8%
2	I	100	40% 49% • 8%

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Mol	Chain	Length	Quality of chain
2	J	100	41% 49% • 8%
2	K	100	39% 51% • 8%
2	L	100	40% 50% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7255 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 receptor superfamily member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	86	710	444	125	136	5	0	0	0
1	B	86	710	444	125	136	5	0	0	0
1	C	86	710	444	125	136	5	0	0	0
1	D	86	710	444	125	136	5	0	0	0
1	E	86	710	444	125	136	5	0	0	0

- Molecule 2 is a protein called Protein FADD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	92	741	453	142	142	4	0	0	0
2	I	92	741	453	142	142	4	0	0	0
2	J	92	741	453	142	142	4	0	0	0
2	K	92	741	453	142	142	4	0	0	0
2	L	92	741	453	142	142	4	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	185	LEU	-	expression tag	UNP Q13158
H	186	GLU	-	expression tag	UNP Q13158
H	187	HIS	-	expression tag	UNP Q13158
H	188	HIS	-	expression tag	UNP Q13158
H	189	HIS	-	expression tag	UNP Q13158

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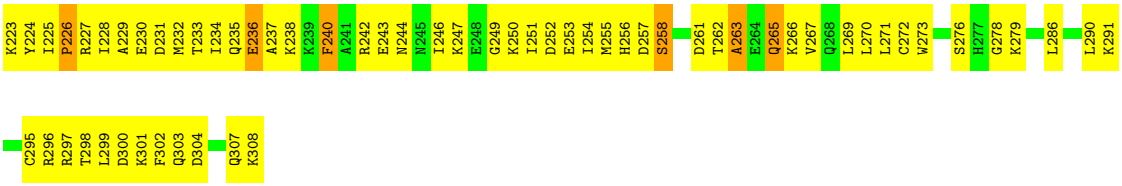
Chain	Residue	Modelled	Actual	Comment	Reference
H	190	HIS	-	expression tag	UNP Q13158
H	191	HIS	-	expression tag	UNP Q13158
H	192	HIS	-	expression tag	UNP Q13158
I	185	LEU	-	expression tag	UNP Q13158
I	186	GLU	-	expression tag	UNP Q13158
I	187	HIS	-	expression tag	UNP Q13158
I	188	HIS	-	expression tag	UNP Q13158
I	189	HIS	-	expression tag	UNP Q13158
I	190	HIS	-	expression tag	UNP Q13158
I	191	HIS	-	expression tag	UNP Q13158
I	192	HIS	-	expression tag	UNP Q13158
J	185	LEU	-	expression tag	UNP Q13158
J	186	GLU	-	expression tag	UNP Q13158
J	187	HIS	-	expression tag	UNP Q13158
J	188	HIS	-	expression tag	UNP Q13158
J	189	HIS	-	expression tag	UNP Q13158
J	190	HIS	-	expression tag	UNP Q13158
J	191	HIS	-	expression tag	UNP Q13158
J	192	HIS	-	expression tag	UNP Q13158
K	185	LEU	-	expression tag	UNP Q13158
K	186	GLU	-	expression tag	UNP Q13158
K	187	HIS	-	expression tag	UNP Q13158
K	188	HIS	-	expression tag	UNP Q13158
K	189	HIS	-	expression tag	UNP Q13158
K	190	HIS	-	expression tag	UNP Q13158
K	191	HIS	-	expression tag	UNP Q13158
K	192	HIS	-	expression tag	UNP Q13158
L	185	LEU	-	expression tag	UNP Q13158
L	186	GLU	-	expression tag	UNP Q13158
L	187	HIS	-	expression tag	UNP Q13158
L	188	HIS	-	expression tag	UNP Q13158
L	189	HIS	-	expression tag	UNP Q13158
L	190	HIS	-	expression tag	UNP Q13158
L	191	HIS	-	expression tag	UNP Q13158
L	192	HIS	-	expression tag	UNP Q13158

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. 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. 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 receptor superfamily member 6

Chain A:

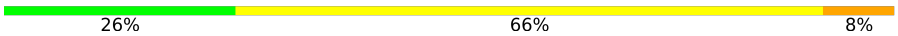


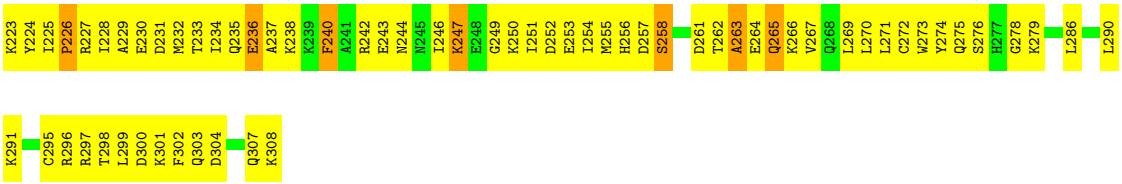
• Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain B:

• Molecule 1: Tumor necrosis factor receptor superfamily member 6

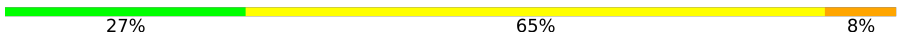
Chain C:

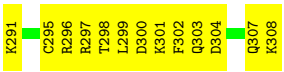




• Molecule 1: Tumor necrosis factor receptor superfamily member 6

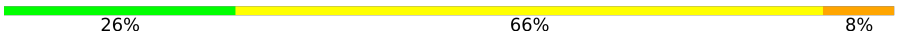
Chain D:

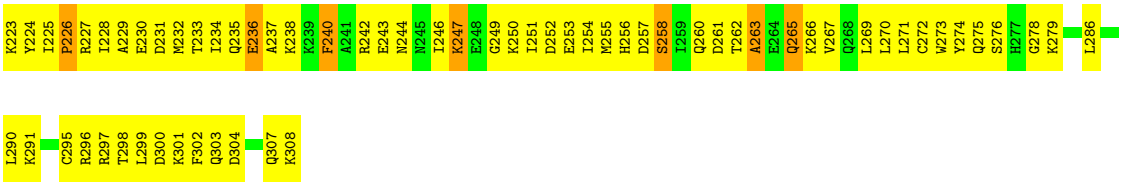




• Molecule 1: Tumor necrosis factor receptor superfamily member 6

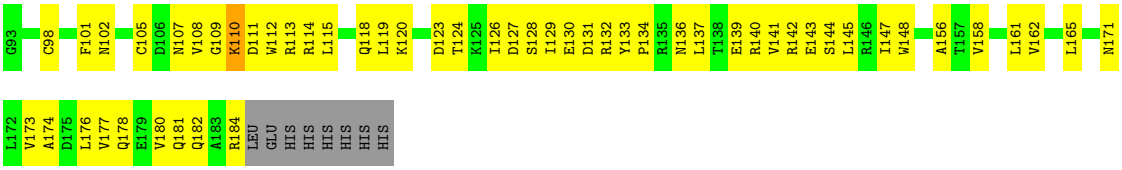
Chain E:





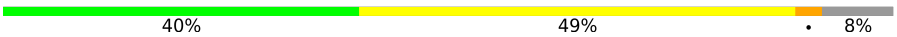
• Molecule 2: Protein FADD

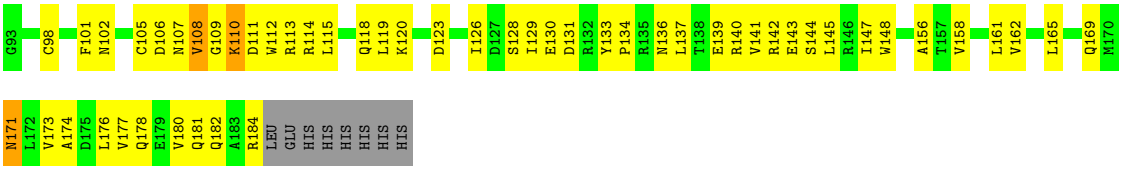
Chain H:



• Molecule 2: Protein FADD

Chain I:



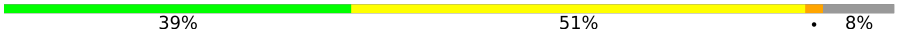


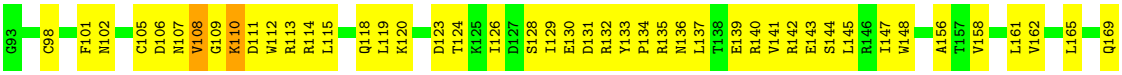
• Molecule 2: Protein FADD

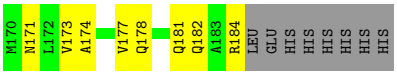
Chain J:

• Molecule 2: Protein FADD

Chain K:

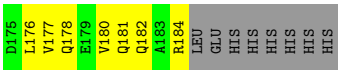






• Molecule 2: Protein FADD

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	135.20Å 144.45Å 131.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 6.80 19.96 – 6.80	Depositor EDS
% Data completeness (in resolution range)	85.6 (20.00-6.80) 85.6 (19.96-6.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 6.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.343 , 0.354 0.385 , 0.358	Depositor DCC
R_{free} test set	105 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	391.5	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 323.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	7255	wwPDB-VP
Average B, all atoms (Å^2)	452.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.41% 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	0.69	0/719	0.85	0/957
1	B	0.69	0/719	0.84	0/957
1	C	0.70	0/719	0.83	0/957
1	D	0.70	0/719	0.84	0/957
1	E	0.69	0/719	0.83	0/957
2	H	0.63	0/748	0.88	0/1008
2	I	0.61	0/748	0.88	0/1008
2	J	0.61	0/748	0.88	0/1008
2	K	0.62	0/748	0.89	0/1008
2	L	0.62	0/748	0.88	0/1008
All	All	0.66	0/7335	0.86	0/9825

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	710	0	717	144	0
1	B	710	0	717	164	0
1	C	710	0	717	174	0
1	D	710	0	717	166	0
1	E	710	0	717	150	0
2	H	741	0	743	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	741	0	743	61	0
2	J	741	0	743	59	0
2	K	741	0	743	64	0
2	L	741	0	743	55	0
All	All	7255	0	7300	1030	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 71.

The worst 5 of 1030 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:C:253:GLU:HB2	1:D:262:THR:CB	1.60	1.29
1:C:257:ASP:O	1:D:260:GLN:HG2	1.41	1.19
1:B:294:GLU:OE1	1:C:230:GLU:HB3	1.39	1.16
1:C:253:GLU:HB2	1:D:262:THR:HB	1.22	1.12
1:E:290:LEU:HD21	1:E:298:THR:HB	1.32	1.11

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	84/86 (98%)	62 (74%)	14 (17%)	8 (10%)	0 10
1	B	84/86 (98%)	62 (74%)	14 (17%)	8 (10%)	0 10
1	C	84/86 (98%)	62 (74%)	14 (17%)	8 (10%)	0 10
1	D	84/86 (98%)	62 (74%)	14 (17%)	8 (10%)	0 10
1	E	84/86 (98%)	62 (74%)	14 (17%)	8 (10%)	0 10
2	H	90/100 (90%)	75 (83%)	13 (14%)	2 (2%)	6 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	90/100 (90%)	73 (81%)	15 (17%)	2 (2%)	6	35
2	J	90/100 (90%)	74 (82%)	14 (16%)	2 (2%)	6	35
2	K	90/100 (90%)	74 (82%)	14 (16%)	2 (2%)	6	35
2	L	90/100 (90%)	73 (81%)	15 (17%)	2 (2%)	6	35
All	All	870/930 (94%)	679 (78%)	141 (16%)	50 (6%)	1	18

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	PHE
1	A	263	ALA
1	B	240	PHE
1	B	263	ALA
1	C	240	PHE

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	77/77 (100%)	76 (99%)	1 (1%)	69	82
1	B	77/77 (100%)	76 (99%)	1 (1%)	69	82
1	C	77/77 (100%)	76 (99%)	1 (1%)	69	82
1	D	77/77 (100%)	76 (99%)	1 (1%)	69	82
1	E	77/77 (100%)	76 (99%)	1 (1%)	69	82
2	H	81/89 (91%)	80 (99%)	1 (1%)	71	83
2	I	81/89 (91%)	80 (99%)	1 (1%)	71	83
2	J	81/89 (91%)	80 (99%)	1 (1%)	71	83
2	K	81/89 (91%)	80 (99%)	1 (1%)	71	83
2	L	81/89 (91%)	80 (99%)	1 (1%)	71	83
All	All	790/830 (95%)	780 (99%)	10 (1%)	69	82

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	171	ASN
2	K	171	ASN
2	L	171	ASN
1	D	236	GLU
1	E	236	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	178	GLN
2	J	160	HIS
2	L	160	HIS
2	J	107	ASN
2	J	178	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.