



wwPDB X-ray Structure Validation Summary Report ⓘ

May 8, 2024 – 04:31 PM JST

PDB ID : 8YD7
Title : Structure of FADD/Caspase-8/cFLIP death effector domain assembly
Authors : Lin, S.-C.; Yang, C.-Y.
Deposited on : 2024-02-19
Resolution : 3.32 Å(reported)

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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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

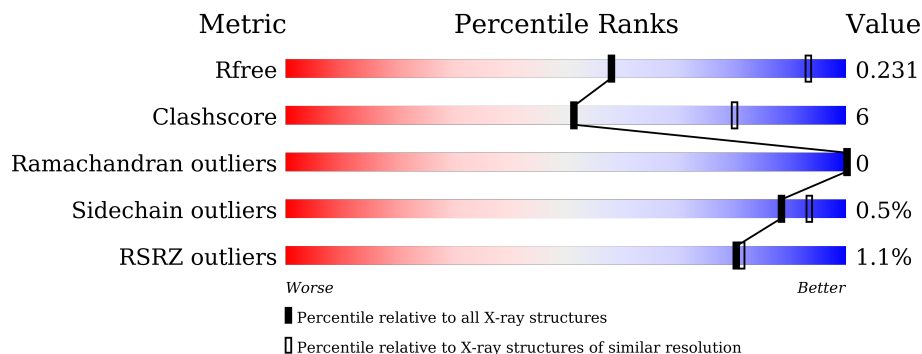
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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.



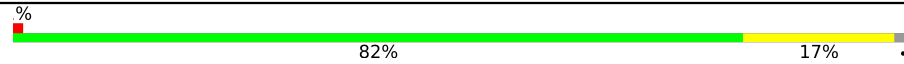
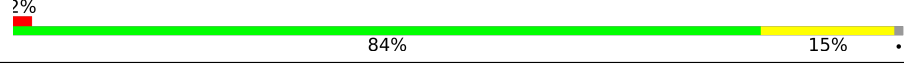
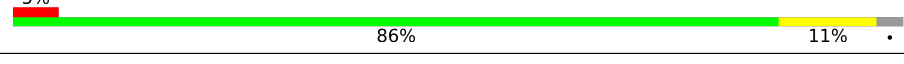

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 $\leq 5\%$. 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	G	181	 79% 15% 6%
1	H	181	 82% 14% 2%
1	I	181	 78% 18% 2%
1	K	181	 83% 11% 6%
2	A	185	 76% 23% 1%
2	B	185	 81% 17% 2%

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Mol	Chain	Length	Quality of chain
2	C	185	 <p>82% 17%</p>
2	D	185	 <p>84% 15%</p>
2	E	185	 <p>86% 11%</p>
3	L	216	 <p>31% 8% 61%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13822 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 CASP8 and FADD-like apoptosis regulator subunit p12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	G	171	1387	882	238	260	2	5	0	0	0
1	H	175	1418	902	245	263	2	6	0	0	0
1	I	175	1418	902	245	263	2	6	0	0	0
1	K	170	1385	882	237	258	2	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	7	GLY	HIS	engineered mutation	UNP O15519
H	7	GLY	HIS	engineered mutation	UNP O15519
I	7	GLY	HIS	engineered mutation	UNP O15519
K	7	GLY	HIS	engineered mutation	UNP O15519

- Molecule 2 is a protein called Caspase-8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	D	183	1519	962	257	291	2	7	0	0	0
2	C	182	1510	956	255	290	2	7	0	0	0
2	B	182	1510	956	255	290	2	7	0	0	0
2	E	180	1496	948	253	287	2	6	0	0	0
2	A	182	1510	956	255	290	2	7	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	122	GLY	PHE	engineered mutation	UNP Q14790
D	123	GLY	LEU	engineered mutation	UNP Q14790
C	122	GLY	PHE	engineered mutation	UNP Q14790
C	123	GLY	LEU	engineered mutation	UNP Q14790
B	122	GLY	PHE	engineered mutation	UNP Q14790
B	123	GLY	LEU	engineered mutation	UNP Q14790
E	122	GLY	PHE	engineered mutation	UNP Q14790
E	123	GLY	LEU	engineered mutation	UNP Q14790
A	122	GLY	PHE	engineered mutation	UNP Q14790
A	123	GLY	LEU	engineered mutation	UNP Q14790

- Molecule 3 is a protein called FAS-associated death domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
3	L	84	668	420	118	127	1	2	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	9	GLY	HIS	engineered mutation	UNP Q13158
L	209	LEU	-	expression tag	UNP Q13158
L	210	GLU	-	expression tag	UNP Q13158
L	211	HIS	-	expression tag	UNP Q13158
L	212	HIS	-	expression tag	UNP Q13158
L	213	HIS	-	expression tag	UNP Q13158
L	214	HIS	-	expression tag	UNP Q13158
L	215	HIS	-	expression tag	UNP Q13158
L	216	HIS	-	expression tag	UNP Q13158


- Molecule 4 is SELENIUM ATOM (three-letter code: SE) (formula: Se).

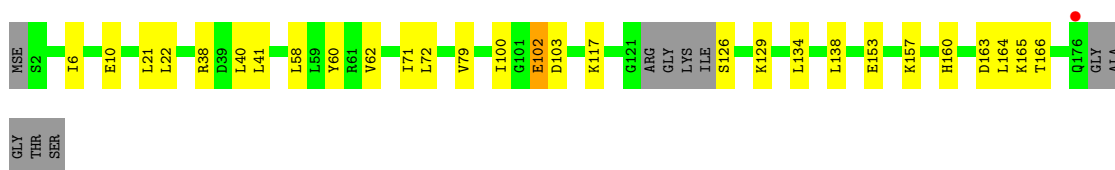
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Se	0	0
			1	1		

3 Residue-property plots


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: CASP8 and FADD-like apoptosis regulator subunit p12

Chain G: 




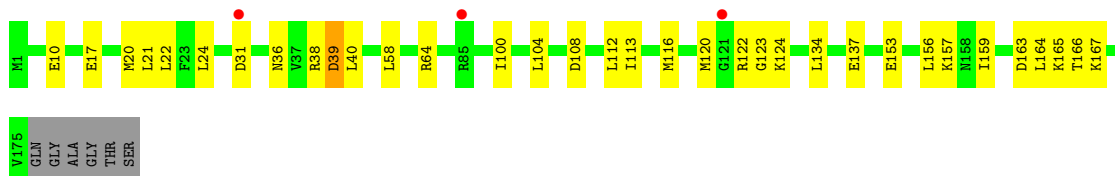
- Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

Chain H: 




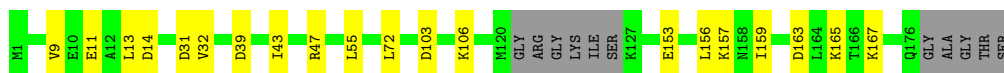
- Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

Chain I: 




- Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

Chain K: 

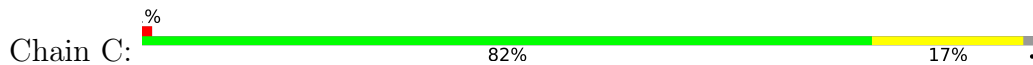


- Molecule 2: Caspase-8

Chain D: 

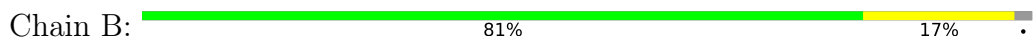


• Molecule 2: Caspase-8



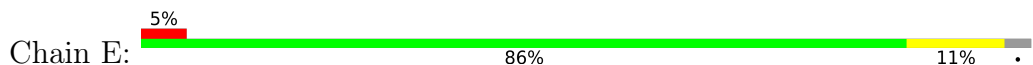
GLU ARG

• Molecule 2: Caspase-8

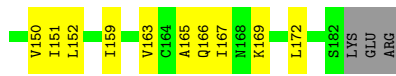


LYS GLU ARG

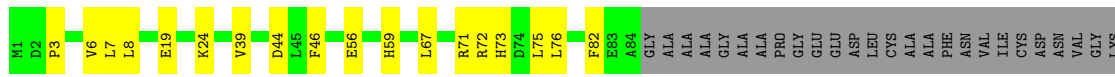
• Molecule 2: Caspase-8



• Molecule 2: Caspase-8



• Molecule 3: FAS-associated death domain protein



ASP TRP ARG ARG LEU ALA ARG GLN LEU LYS VAL SER ASP THR LYS ILE ASP SER ILE GLU ASP ARG TYR PRO ASN THR LEU THR ARG VAL ASP THR LEU CYS ALA HIS LEU VAL VAL GLY ALA LEU CYS ASP ASN VAL CYS GLN MSE

ASN
LEU
VAL
ALA
ASP
LEU
VAL
GLN
GLU
VAL
GLN
GLN
ALA
ARG
ASP
LEU
GLN
ASN
ARG
SER
GLY
ALA
MSE
SER
PRO
MSE
SER
TRP
ASN
SER
ASP
ALA
SER
THR
SER
GLU
ALA
SER
LEU
GLU
HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.94Å 150.06Å 175.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 3.32 29.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.81-3.32) 99.0 (29.81-3.32)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.19 (at 3.31Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.231 0.195 , 0.231	Depositor DCC
R_{free} test set	2200 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	100.8	Xtrriage
Anisotropy	0.783	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13822	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SE

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	G	0.23	0/1395	0.46	0/1864
1	H	0.22	0/1427	0.46	0/1906
1	I	0.22	0/1427	0.45	0/1906
1	K	0.22	0/1393	0.44	0/1861
2	A	0.23	0/1520	0.48	0/2021
2	B	0.23	0/1520	0.45	0/2021
2	C	0.23	0/1520	0.46	0/2021
2	D	0.23	0/1529	0.45	0/2032
2	E	0.23	0/1506	0.46	0/2003
3	L	0.23	0/674	0.52	0/902
All	All	0.23	0/13911	0.46	0/18537

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	G	1387	0	1458	18	0
1	H	1418	0	1503	17	0
1	I	1418	0	1503	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1385	0	1462	13	0
2	A	1510	0	1551	31	0
2	B	1510	0	1551	19	0
2	C	1510	0	1551	17	0
2	D	1519	0	1564	14	0
2	E	1496	0	1534	11	0
3	L	668	0	691	12	0
4	G	1	0	0	0	0
All	All	13822	0	14368	159	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 6.

The worst 5 of 159 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)
2:A:23:LYS:HE3	2:A:35:GLN:HG2	1.68	0.73
1:G:153:GLU:HG2	1:G:165:LYS:HG3	1.72	0.72
2:E:138:ASN:ND2	2:E:141:ASP:OD2	2.23	0.71
2:C:138:ASN:ND2	2:C:141:ASP:OD2	2.24	0.71
1:H:100:ILE:HG23	1:H:164:LEU:HD13	1.72	0.69

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	G	167/181 (92%)	160 (96%)	7 (4%)	0	100 100
1	H	173/181 (96%)	164 (95%)	9 (5%)	0	100 100
1	I	173/181 (96%)	164 (95%)	9 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	166/181 (92%)	159 (96%)	7 (4%)	0	100	100
2	A	180/185 (97%)	176 (98%)	4 (2%)	0	100	100
2	B	180/185 (97%)	175 (97%)	5 (3%)	0	100	100
2	C	180/185 (97%)	177 (98%)	3 (2%)	0	100	100
2	D	181/185 (98%)	177 (98%)	4 (2%)	0	100	100
2	E	178/185 (96%)	174 (98%)	4 (2%)	0	100	100
3	L	82/216 (38%)	80 (98%)	2 (2%)	0	100	100
All	All	1660/1865 (89%)	1606 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	G	159/159 (100%)	158 (99%)	1 (1%)	86	92
1	H	162/159 (102%)	161 (99%)	1 (1%)	86	92
1	I	162/159 (102%)	161 (99%)	1 (1%)	86	92
1	K	159/159 (100%)	158 (99%)	1 (1%)	86	92
2	A	171/167 (102%)	171 (100%)	0	100	100
2	B	171/167 (102%)	170 (99%)	1 (1%)	86	92
2	C	171/167 (102%)	169 (99%)	2 (1%)	71	84
2	D	172/167 (103%)	171 (99%)	1 (1%)	86	92
2	E	169/167 (101%)	169 (100%)	0	100	100
3	L	77/182 (42%)	77 (100%)	0	100	100
All	All	1573/1653 (95%)	1565 (100%)	8 (0%)	88	93

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	39	ASP
1	I	39	ASP
2	B	136	ASP
2	C	158	ASP
1	H	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [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	G	166/181 (91%)	-0.08	1 (0%) 89 90	79, 106, 136, 164	0
1	H	169/181 (93%)	-0.11	1 (0%) 89 90	77, 113, 161, 202	0
1	I	169/181 (93%)	-0.20	3 (1%) 68 67	82, 104, 138, 165	0
1	K	164/181 (90%)	-0.21	0 100 100	78, 98, 136, 161	0
2	A	175/185 (94%)	-0.17	0 100 100	76, 99, 136, 143	0
2	B	175/185 (94%)	-0.05	0 100 100	82, 108, 149, 168	0
2	C	175/185 (94%)	-0.17	1 (0%) 89 90	80, 111, 150, 174	0
2	D	176/185 (95%)	-0.14	3 (1%) 70 68	82, 116, 152, 184	0
2	E	174/185 (94%)	0.07	9 (5%) 27 27	91, 122, 160, 181	0
3	L	82/216 (37%)	-0.38	0 100 100	84, 104, 131, 140	0
All	All	1625/1865 (87%)	-0.13	18 (1%) 80 81	76, 108, 150, 202	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	120	PHE	3.3
1	I	121	GLY	3.3
2	E	93	PRO	2.5
2	C	95	ARG	2.5
1	G	176	GLN	2.5

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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
4	SE	G	201	1/1	0.91	0.27	175,175,175,175	0

6.5 Other polymers [i](#)

There are no such residues in this entry.