wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:51 AM GMT

PDB ID	:	2OF5
Title	:	Oligomeric Death Domain complex
Authors	:	Park, H.H.; Logette, E.; Raunser, S.; Cuenin, S.; Walz, T.; Tschopp, J.; Wu, H.
Deposited on	:	2007-01-02
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/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:

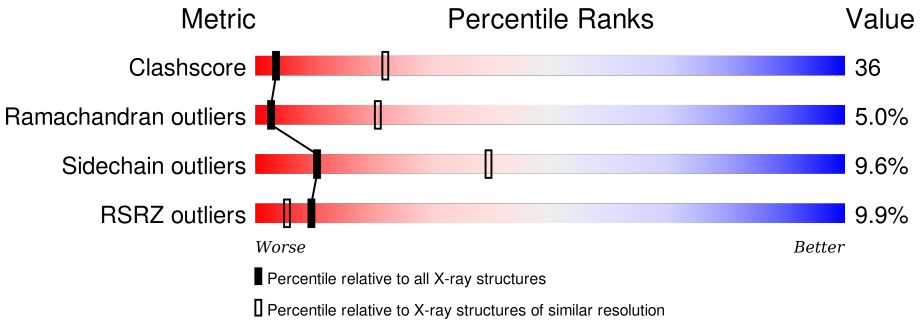
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	114	2% 35% 41% • 20%
1	B	114	2% 39% 33% 7% 20%
1	C	114	% 39% 38% • 20%
1	D	114	39% 39% • 20%
1	E	114	31% 42% 7% 20%
1	F	114	34% 33% 42% • 20%
1	G	114	54% 24% 49% 7% 20%

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Mol	Chain	Length	Quality of chain
2	H	118	32% 39% 13% 15%
2	I	118	2% 38% 38% 8% 15%
2	J	118	% 41% 36% 8% 15%
2	K	118	2% 36% 36% 14% 15%
2	L	118	% 33% 43% 8% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9117 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 Death domain-containing protein CRADD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			
1	B	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			
1	C	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			
1	D	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			
1	E	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			
1	F	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			
1	G	91	Total	C	N	O	S	0	0	0
			738	463	140	132	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	LEU	-	CLONING ARTIFACT	UNP P78560
A	201	GLU	-	CLONING ARTIFACT	UNP P78560
A	202	HIS	-	EXPRESSION TAG	UNP P78560
A	203	HIS	-	EXPRESSION TAG	UNP P78560
A	204	HIS	-	EXPRESSION TAG	UNP P78560
A	205	HIS	-	EXPRESSION TAG	UNP P78560
A	206	HIS	-	EXPRESSION TAG	UNP P78560
A	207	HIS	-	EXPRESSION TAG	UNP P78560
B	200	LEU	-	CLONING ARTIFACT	UNP P78560
B	201	GLU	-	CLONING ARTIFACT	UNP P78560
B	202	HIS	-	EXPRESSION TAG	UNP P78560
B	203	HIS	-	EXPRESSION TAG	UNP P78560
B	204	HIS	-	EXPRESSION TAG	UNP P78560
B	205	HIS	-	EXPRESSION TAG	UNP P78560
B	206	HIS	-	EXPRESSION TAG	UNP P78560

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	HIS	-	EXPRESSION TAG	UNP P78560
C	200	LEU	-	CLONING ARTIFACT	UNP P78560
C	201	GLU	-	CLONING ARTIFACT	UNP P78560
C	202	HIS	-	EXPRESSION TAG	UNP P78560
C	203	HIS	-	EXPRESSION TAG	UNP P78560
C	204	HIS	-	EXPRESSION TAG	UNP P78560
C	205	HIS	-	EXPRESSION TAG	UNP P78560
C	206	HIS	-	EXPRESSION TAG	UNP P78560
C	207	HIS	-	EXPRESSION TAG	UNP P78560
D	200	LEU	-	CLONING ARTIFACT	UNP P78560
D	201	GLU	-	CLONING ARTIFACT	UNP P78560
D	202	HIS	-	EXPRESSION TAG	UNP P78560
D	203	HIS	-	EXPRESSION TAG	UNP P78560
D	204	HIS	-	EXPRESSION TAG	UNP P78560
D	205	HIS	-	EXPRESSION TAG	UNP P78560
D	206	HIS	-	EXPRESSION TAG	UNP P78560
D	207	HIS	-	EXPRESSION TAG	UNP P78560
E	200	LEU	-	CLONING ARTIFACT	UNP P78560
E	201	GLU	-	CLONING ARTIFACT	UNP P78560
E	202	HIS	-	EXPRESSION TAG	UNP P78560
E	203	HIS	-	EXPRESSION TAG	UNP P78560
E	204	HIS	-	EXPRESSION TAG	UNP P78560
E	205	HIS	-	EXPRESSION TAG	UNP P78560
E	206	HIS	-	EXPRESSION TAG	UNP P78560
E	207	HIS	-	EXPRESSION TAG	UNP P78560
F	200	LEU	-	CLONING ARTIFACT	UNP P78560
F	201	GLU	-	CLONING ARTIFACT	UNP P78560
F	202	HIS	-	EXPRESSION TAG	UNP P78560
F	203	HIS	-	EXPRESSION TAG	UNP P78560
F	204	HIS	-	EXPRESSION TAG	UNP P78560
F	205	HIS	-	EXPRESSION TAG	UNP P78560
F	206	HIS	-	EXPRESSION TAG	UNP P78560
F	207	HIS	-	EXPRESSION TAG	UNP P78560
G	200	LEU	-	CLONING ARTIFACT	UNP P78560
G	201	GLU	-	CLONING ARTIFACT	UNP P78560
G	202	HIS	-	EXPRESSION TAG	UNP P78560
G	203	HIS	-	EXPRESSION TAG	UNP P78560
G	204	HIS	-	EXPRESSION TAG	UNP P78560
G	205	HIS	-	EXPRESSION TAG	UNP P78560
G	206	HIS	-	EXPRESSION TAG	UNP P78560
G	207	HIS	-	EXPRESSION TAG	UNP P78560

- Molecule 2 is a protein called Leucine-rich repeat and death domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	100	Total	C	N	O	S	0	0	0
			786	489	145	150	2			
2	I	100	Total	C	N	O	S	0	0	0
			786	489	145	150	2			
2	J	100	Total	C	N	O	S	0	0	0
			786	489	145	150	2			
2	K	100	Total	C	N	O	S	0	0	0
			786	489	145	150	2			
2	L	100	Total	C	N	O	S	0	0	0
			786	489	145	150	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	777	MET	-	CLONING ARTIFACT	UNP Q9HB75
H	884	ALA	-	CLONING ARTIFACT	UNP Q9HB75
H	885	ALA	-	CLONING ARTIFACT	UNP Q9HB75
H	886	ALA	-	CLONING ARTIFACT	UNP Q9HB75
H	887	LEU	-	CLONING ARTIFACT	UNP Q9HB75
H	888	GLU	-	CLONING ARTIFACT	UNP Q9HB75
H	889	HIS	-	EXPRESSION TAG	UNP Q9HB75
H	890	HIS	-	EXPRESSION TAG	UNP Q9HB75
H	891	HIS	-	EXPRESSION TAG	UNP Q9HB75
H	892	HIS	-	EXPRESSION TAG	UNP Q9HB75
H	893	HIS	-	EXPRESSION TAG	UNP Q9HB75
H	894	HIS	-	EXPRESSION TAG	UNP Q9HB75
I	777	MET	-	CLONING ARTIFACT	UNP Q9HB75
I	884	ALA	-	CLONING ARTIFACT	UNP Q9HB75
I	885	ALA	-	CLONING ARTIFACT	UNP Q9HB75
I	886	ALA	-	CLONING ARTIFACT	UNP Q9HB75
I	887	LEU	-	CLONING ARTIFACT	UNP Q9HB75
I	888	GLU	-	CLONING ARTIFACT	UNP Q9HB75
I	889	HIS	-	EXPRESSION TAG	UNP Q9HB75
I	890	HIS	-	EXPRESSION TAG	UNP Q9HB75
I	891	HIS	-	EXPRESSION TAG	UNP Q9HB75
I	892	HIS	-	EXPRESSION TAG	UNP Q9HB75
I	893	HIS	-	EXPRESSION TAG	UNP Q9HB75
I	894	HIS	-	EXPRESSION TAG	UNP Q9HB75
J	777	MET	-	CLONING ARTIFACT	UNP Q9HB75
J	884	ALA	-	CLONING ARTIFACT	UNP Q9HB75
J	885	ALA	-	CLONING ARTIFACT	UNP Q9HB75
J	886	ALA	-	CLONING ARTIFACT	UNP Q9HB75
J	887	LEU	-	CLONING ARTIFACT	UNP Q9HB75
J	888	GLU	-	CLONING ARTIFACT	UNP Q9HB75

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Chain	Residue	Modelled	Actual	Comment	Reference
J	889	HIS	-	EXPRESSION TAG	UNP Q9HB75
J	890	HIS	-	EXPRESSION TAG	UNP Q9HB75
J	891	HIS	-	EXPRESSION TAG	UNP Q9HB75
J	892	HIS	-	EXPRESSION TAG	UNP Q9HB75
J	893	HIS	-	EXPRESSION TAG	UNP Q9HB75
J	894	HIS	-	EXPRESSION TAG	UNP Q9HB75
K	777	MET	-	CLONING ARTIFACT	UNP Q9HB75
K	884	ALA	-	CLONING ARTIFACT	UNP Q9HB75
K	885	ALA	-	CLONING ARTIFACT	UNP Q9HB75
K	886	ALA	-	CLONING ARTIFACT	UNP Q9HB75
K	887	LEU	-	CLONING ARTIFACT	UNP Q9HB75
K	888	GLU	-	CLONING ARTIFACT	UNP Q9HB75
K	889	HIS	-	EXPRESSION TAG	UNP Q9HB75
K	890	HIS	-	EXPRESSION TAG	UNP Q9HB75
K	891	HIS	-	EXPRESSION TAG	UNP Q9HB75
K	892	HIS	-	EXPRESSION TAG	UNP Q9HB75
K	893	HIS	-	EXPRESSION TAG	UNP Q9HB75
K	894	HIS	-	EXPRESSION TAG	UNP Q9HB75
L	777	MET	-	CLONING ARTIFACT	UNP Q9HB75
L	884	ALA	-	CLONING ARTIFACT	UNP Q9HB75
L	885	ALA	-	CLONING ARTIFACT	UNP Q9HB75
L	886	ALA	-	CLONING ARTIFACT	UNP Q9HB75
L	887	LEU	-	CLONING ARTIFACT	UNP Q9HB75
L	888	GLU	-	CLONING ARTIFACT	UNP Q9HB75
L	889	HIS	-	EXPRESSION TAG	UNP Q9HB75
L	890	HIS	-	EXPRESSION TAG	UNP Q9HB75
L	891	HIS	-	EXPRESSION TAG	UNP Q9HB75
L	892	HIS	-	EXPRESSION TAG	UNP Q9HB75
L	893	HIS	-	EXPRESSION TAG	UNP Q9HB75
L	894	HIS	-	EXPRESSION TAG	UNP Q9HB75

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	1	Total O 1 1	0	0
3	C	3	Total O 3 3	0	0
3	D	2	Total O 2 2	0	0

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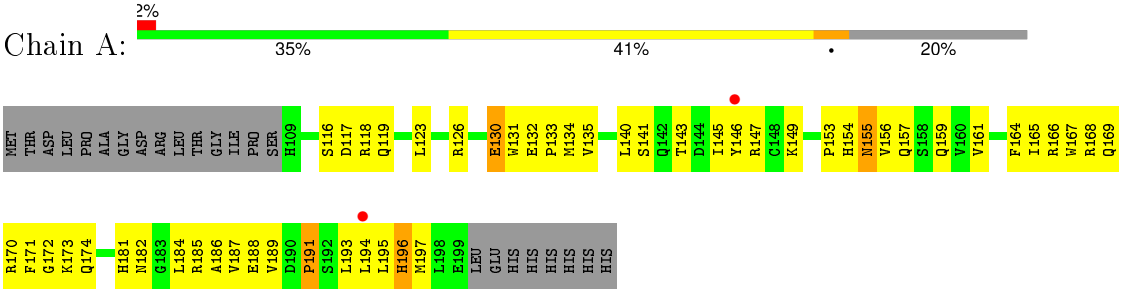
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total O 2 2	0	0
3	H	5	Total O 5 5	0	0
3	J	3	Total O 3 3	0	0
3	K	3	Total O 3 3	0	0

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 errors 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.

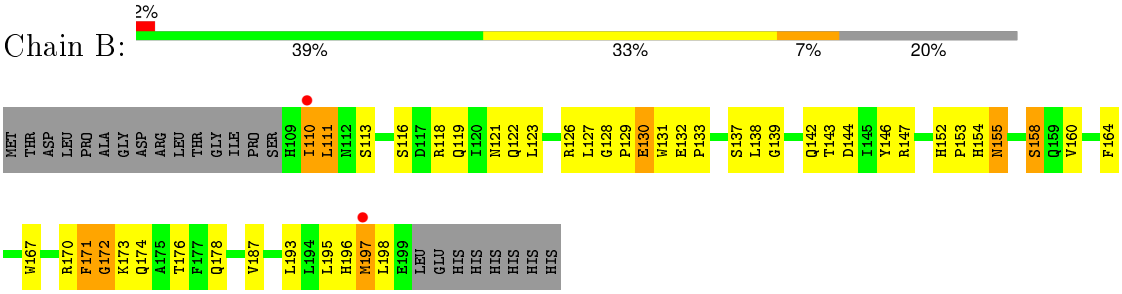
- Molecule 1: Death domain-containing protein CRADD

Chain A:



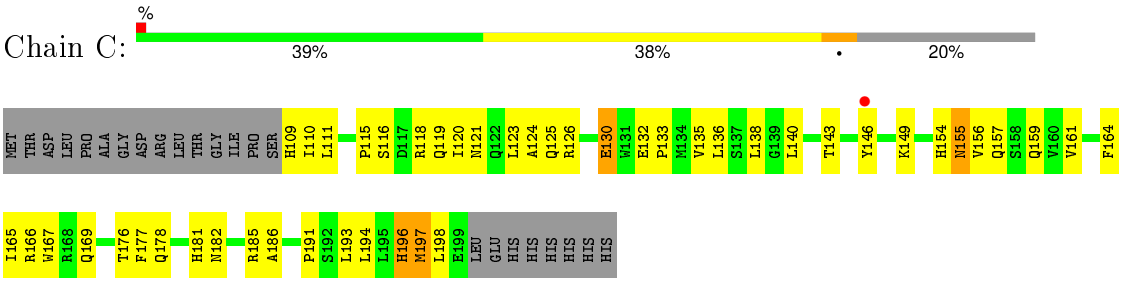
- Molecule 1: Death domain-containing protein CRADD

Chain B:



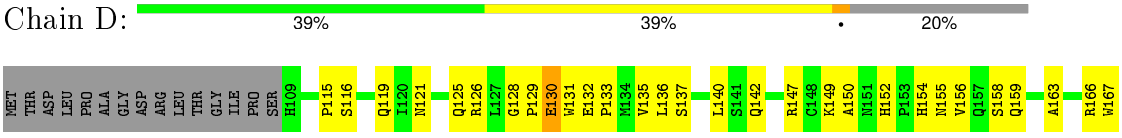
- Molecule 1: Death domain-containing protein CRADD

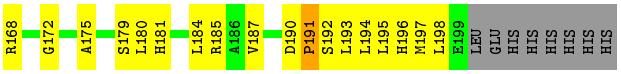
Chain C:



- Molecule 1: Death domain-containing protein CRADD

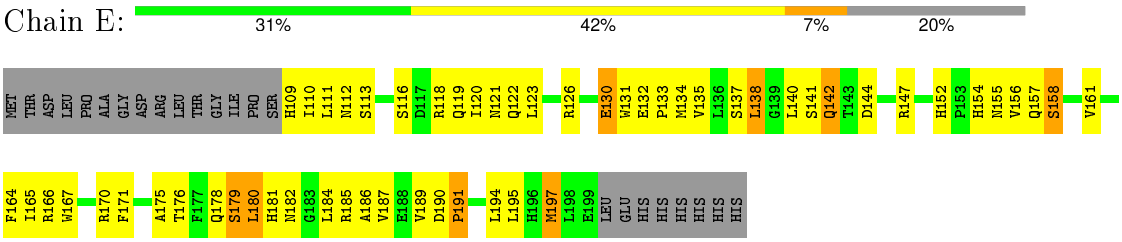
Chain D:





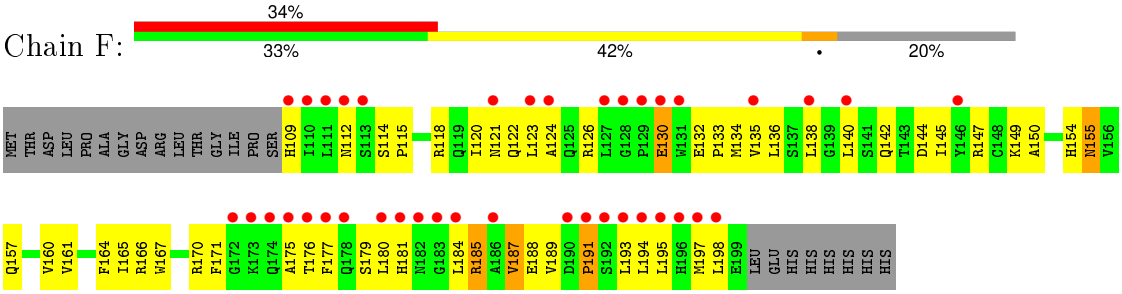
• Molecule 1: Death domain-containing protein CRADD

Chain E:



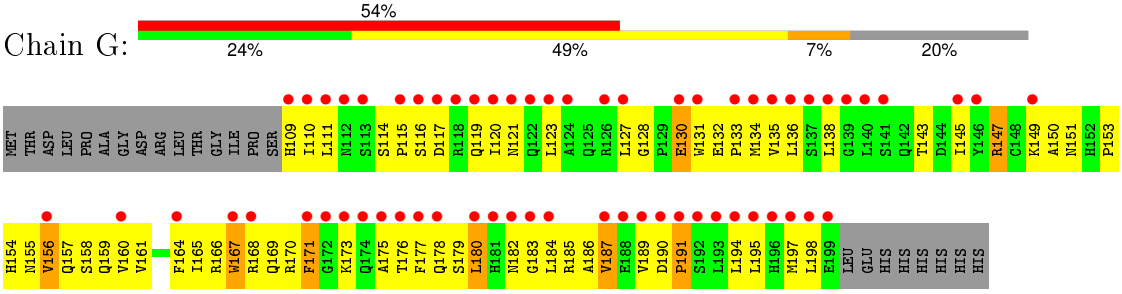
• Molecule 1: Death domain-containing protein CRADD

Chain F:



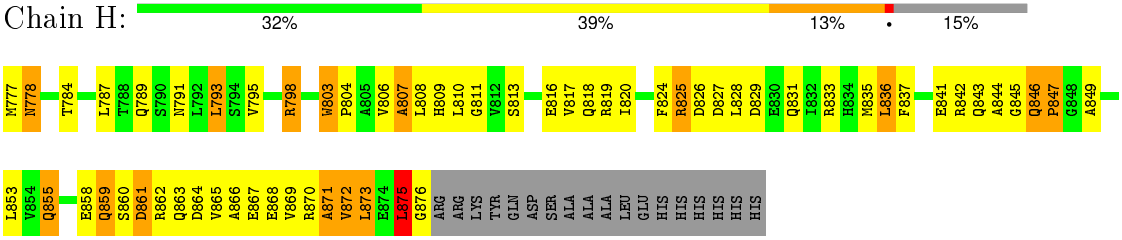
• Molecule 1: Death domain-containing protein CRADD

Chain G:



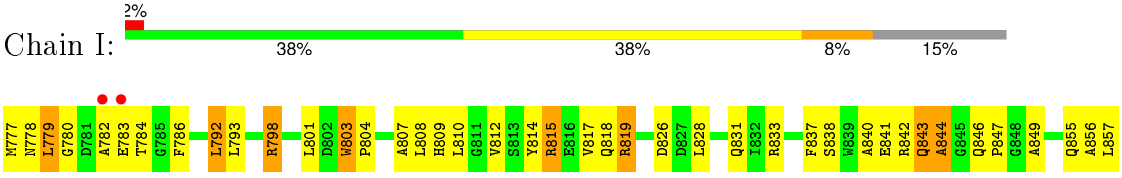
• Molecule 2: Leucine-rich repeat and death domain-containing protein

Chain H:



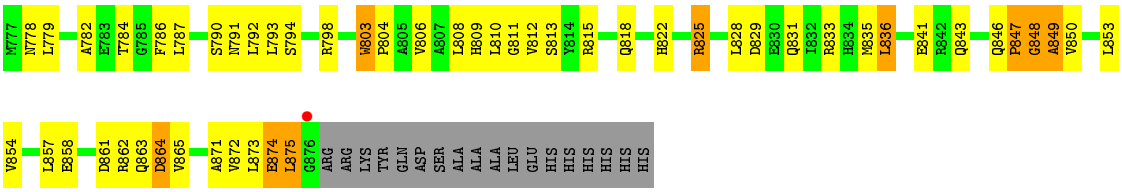
• Molecule 2: Leucine-rich repeat and death domain-containing protein

Chain I:



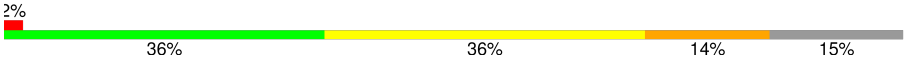
- Molecule 2: Leucine-rich repeat and death domain-containing protein

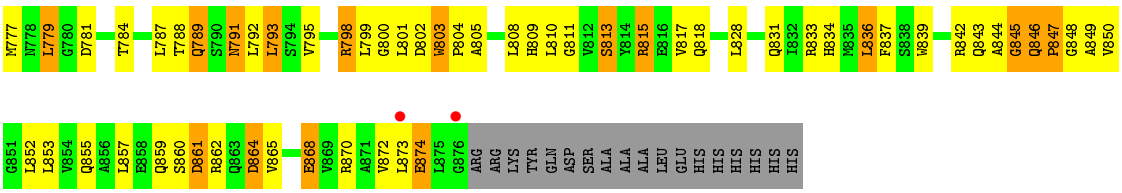
Chain J:



- Molecule 2: Leucine-rich repeat and death domain-containing protein

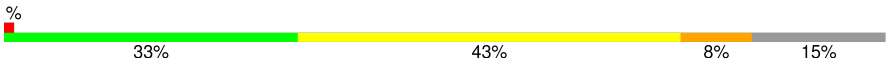
Chain K:

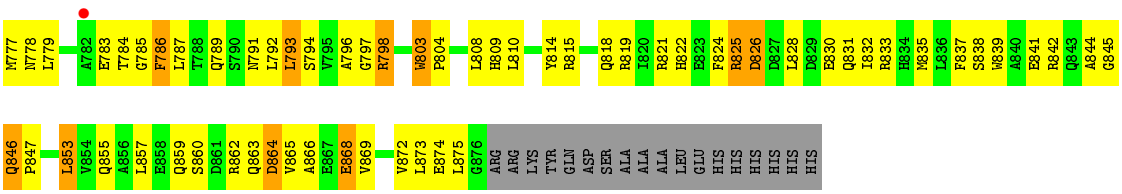




- Molecule 2: Leucine-rich repeat and death domain-containing protein

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	138.40Å 138.40Å 207.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.20 45.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 93.4 (45.29-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.275 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	92.0	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.5	EDS
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 36209 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9117	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0/755	0.60	0/1023
1	B	0.46	0/755	0.66	0/1023
1	C	0.47	0/755	0.66	0/1023
1	D	0.45	0/755	0.63	0/1023
1	E	0.40	0/755	0.63	0/1023
1	F	0.30	0/755	0.52	0/1023
1	G	1.46	6/755 (0.8%)	3.95	8/1023 (0.8%)
2	H	0.48	0/798	0.68	0/1079
2	I	0.42	0/798	0.68	0/1079
2	J	0.52	0/798	0.72	0/1079
2	K	0.47	0/798	0.73	0/1079
2	L	0.41	0/798	0.63	0/1079
All	All	0.59	6/9275 (0.1%)	1.29	8/12556 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	171	PHE	CD2-CE2	19.85	1.78	1.39
1	G	171	PHE	CD1-CE1	19.72	1.78	1.39
1	G	171	PHE	CE1-CZ	-16.62	1.05	1.37
1	G	171	PHE	CE2-CZ	-16.58	1.05	1.37
1	G	171	PHE	CG-CD1	10.22	1.54	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	171	PHE	CD1-CE1-CZ	-69.73	36.43	120.10
1	G	171	PHE	CZ-CE2-CD2	-69.40	36.83	120.10
1	G	171	PHE	CE1-CZ-CE2	-53.36	23.95	120.00
1	G	171	PHE	CG-CD1-CE1	-32.94	84.57	120.80
1	G	171	PHE	CG-CD2-CE2	-32.88	84.63	120.80

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	738	0	730	61	0
1	B	738	0	730	47	0
1	C	738	0	730	48	0
1	D	738	0	730	49	0
1	E	738	0	730	63	0
1	F	738	0	730	67	0
1	G	738	0	730	70	0
2	H	786	0	767	75	0
2	I	786	0	767	45	0
2	J	786	0	767	51	0
2	K	786	0	767	70	0
2	L	786	0	767	61	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	H	5	0	0	1	0
3	J	3	0	0	0	0
3	K	3	0	0	2	0
All	All	9117	0	8945	654	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 36.

The worst 5 of 654 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:D:133:PRO:HG3	1:F:157:GLN:HG2	1.43	1.00
1:E:155:ASN:ND2	1:E:158:SER:HB2	1.77	1.00
1:E:135:VAL:HB	1:E:140:LEU:HD12	1.47	0.96
2:H:803:TRP:HZ3	2:H:831:GLN:HE21	1.15	0.95
1:F:171:PHE:HB2	1:F:175:ALA:HB2	1.51	0.93

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	89/114 (78%)	74 (83%)	12 (14%)	3 (3%)	5 31
1	B	89/114 (78%)	78 (88%)	8 (9%)	3 (3%)	5 31
1	C	89/114 (78%)	77 (86%)	10 (11%)	2 (2%)	8 45
1	D	89/114 (78%)	66 (74%)	21 (24%)	2 (2%)	8 45
1	E	89/114 (78%)	79 (89%)	8 (9%)	2 (2%)	8 45
1	F	89/114 (78%)	76 (85%)	10 (11%)	3 (3%)	5 31
1	G	89/114 (78%)	64 (72%)	21 (24%)	4 (4%)	3 24
2	H	98/118 (83%)	77 (79%)	10 (10%)	11 (11%)	0 3
2	I	98/118 (83%)	73 (74%)	18 (18%)	7 (7%)	1 10
2	J	98/118 (83%)	76 (78%)	15 (15%)	7 (7%)	1 10
2	K	98/118 (83%)	82 (84%)	11 (11%)	5 (5%)	2 20
2	L	98/118 (83%)	80 (82%)	11 (11%)	7 (7%)	1 10
All	All	1113/1388 (80%)	902 (81%)	155 (14%)	56 (5%)	3 21

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	F	155	ASN
2	H	778	ASN
2	H	844	ALA
2	H	847	PRO

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	82/102 (80%)	79 (96%)	3 (4%)	41 79
1	B	82/102 (80%)	75 (92%)	7 (8%)	13 47
1	C	82/102 (80%)	77 (94%)	5 (6%)	23 64
1	D	82/102 (80%)	79 (96%)	3 (4%)	41 79
1	E	82/102 (80%)	72 (88%)	10 (12%)	6 27
1	F	82/102 (80%)	76 (93%)	6 (7%)	17 57
1	G	82/102 (80%)	75 (92%)	7 (8%)	13 47
2	H	81/96 (84%)	71 (88%)	10 (12%)	6 27
2	I	81/96 (84%)	70 (86%)	11 (14%)	5 22
2	J	81/96 (84%)	73 (90%)	8 (10%)	10 38
2	K	81/96 (84%)	68 (84%)	13 (16%)	3 14
2	L	81/96 (84%)	70 (86%)	11 (14%)	5 22
All	All	979/1194 (82%)	885 (90%)	94 (10%)	10 39

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	798	ARG
2	I	792	LEU
2	L	798	ARG
2	H	803	TRP
2	H	859	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	169	GLN
1	G	121	ASN
2	L	778	ASN
1	E	178	GLN

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Mol	Chain	Res	Type
1	F	169	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 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	91/114 (79%)	0.07	2 (2%) 65 50	79, 113, 155, 168	0
1	B	91/114 (79%)	0.17	2 (2%) 65 50	77, 104, 141, 163	0
1	C	91/114 (79%)	0.05	1 (1%) 82 72	73, 92, 120, 148	0
1	D	91/114 (79%)	-0.07	0 100 100	73, 97, 132, 154	0
1	E	91/114 (79%)	0.09	0 100 100	82, 104, 148, 174	0
1	F	91/114 (79%)	1.86	39 (42%) 0 0	148, 175, 199, 200	0
1	G	91/114 (79%)	3.02	62 (68%) 0 0	186, 199, 200, 200	0
2	H	100/118 (84%)	-0.19	0 100 100	78, 98, 129, 137	0
2	I	100/118 (84%)	-0.05	2 (2%) 68 54	82, 114, 170, 182	0
2	J	100/118 (84%)	-0.10	1 (1%) 84 75	71, 92, 120, 130	0
2	K	100/118 (84%)	-0.09	2 (2%) 68 54	75, 90, 111, 147	0
2	L	100/118 (84%)	-0.11	1 (1%) 84 75	89, 111, 161, 167	0
All	All	1137/1388 (81%)	0.37	112 (9%) 9 5	71, 105, 198, 200	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	180	LEU	9.5
1	G	173	LYS	9.0
1	G	197	MET	7.1
1	G	172	GLY	7.1
1	G	195	LEU	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 (i)

There are no carbohydrates 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.