



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:25 pm GMT

PDB ID : 2A5Y
Title : Structure of a CED-4/CED-9 complex
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Deposited on : 2005-07-01
Resolution : 2.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

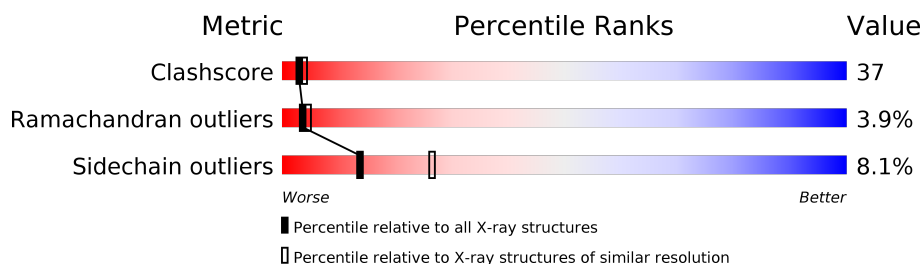
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	204	
2	B	549	
2	C	549	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8730 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 Apoptosis regulator ced-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1417	900	246	262	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	SER	CYS	ENGINEERED	UNP P41958
A	135	SER	CYS	ENGINEERED	UNP P41958
A	164	SER	CYS	ENGINEERED	UNP P41958

- Molecule 2 is a protein called ced-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	501	Total	C	N	O	S	0	0	0
			4028	2568	674	757	29			
2	C	373	Total	C	N	O	S	0	0	0
			2961	1885	493	558	25			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is water.

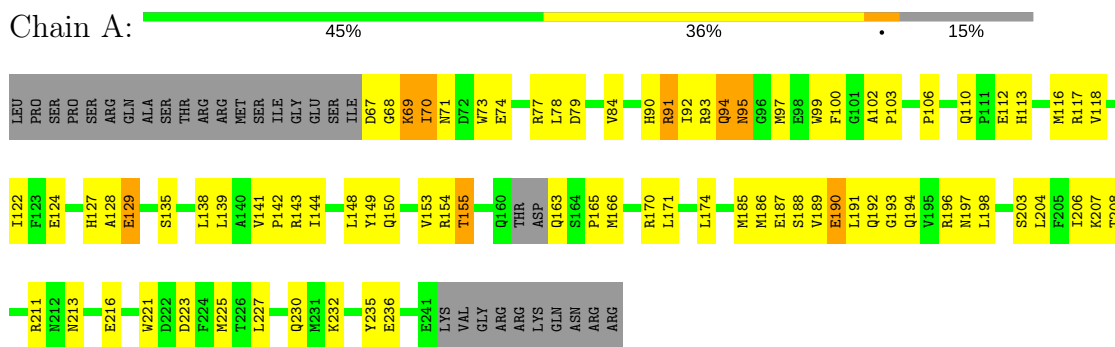
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	145	Total O 145 145	0	0
5	C	83	Total O 83 83	0	0

3 Residue-property plots

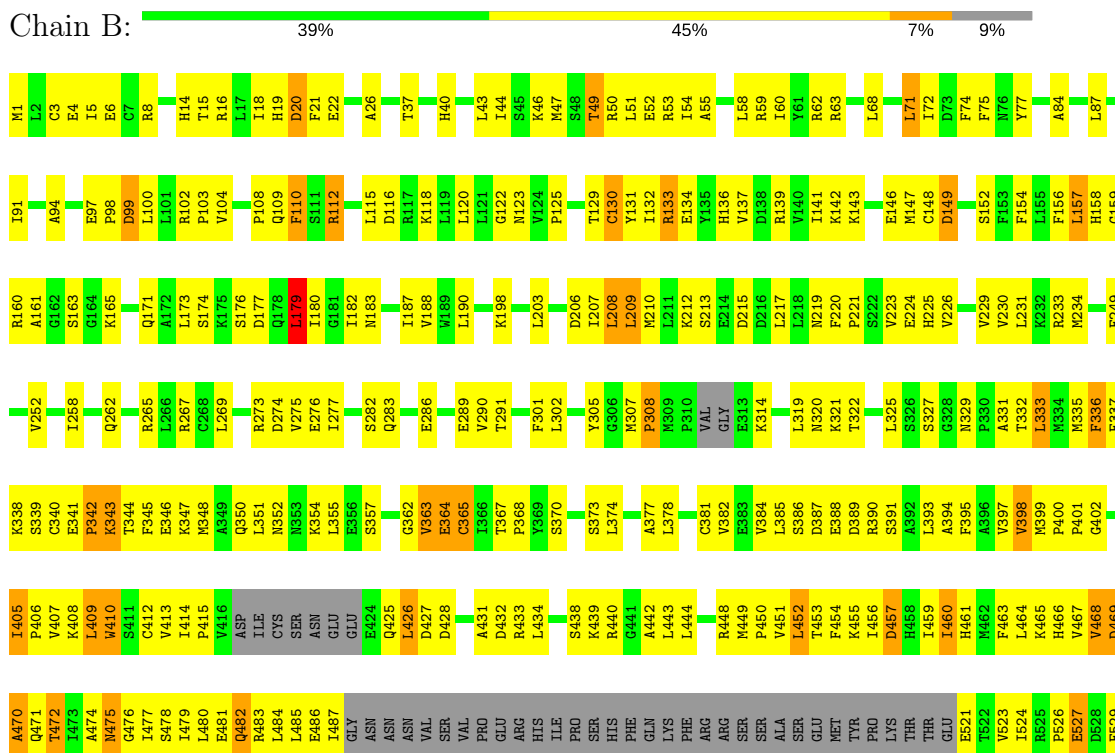
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: Apoptosis regulator ced-9



• Molecule 2: ced-4



P530	K631	F532	M533	Q534	L535	H536	Q537	K538	F539	Y540	D541	S542	L543	LYS	ASN	PHE	ALA	CYS	CYS
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● Molecule 2: ced-4



PHE	ARG	ARG	SER	SER	ALA	SER	GLU	MET	TYR	PRO	LYS	THR	THR	GLU	GLU	VAL	ILE	ARG	PRO	PRO	GLU	ASP	PHE	PRO	LYS	PHE	M533	Q534	L535	H536	Q537	Y540	D541	S542	L543	LYS	ASN	PHE	ALA	CYS																	
L443	L444	K447	R448	M449	P450	V451	L452	T453	F454	K455	I456	I459	I460	H461	V462	F463	L464	V467	V468	D469	A470	Q471	T472	I473	A474	M475	G476	I477	S478	T479	L480	E481	D482	ARG	LEU	LEU	GLU	ILE	GLY	ASN	ASN	VAL	SER	VAL	PRO	GLU	ARG	HIS	ILE	PRO	SER	HIS	PHE	GLN	LYS		
V382	E383	V384	L385	S386	D387	E388	D389	R390	S391	A392	L393	A394	F395	A396	V397	S398	M399	P400	P401	G402	V403	D404	I405	P406	V407	K408	L409	W410	S411	C412	V413	I414	PRO	VAL	ASP	ILE	CYS	SER	ASN	GLU	GLY	GLN	LEU	D427	D428	E429	V430	A431	D432	R433	L434	K435	R436	L437	S438	K439	R440
C298	Y299	L302	Y305	G306	K307	P308	M309	P310	L319	I323	S327	G328	N329	P330	A331	L332	L333	K334	K335	F336	F337	K338	S339	C340	E341	P342	K343	T344	F345	K348	A349	Q350	N353	K354	L355	E356	V361	G362	V363	E364	C365	I366	T367	Y369	L374	Q379	R380	C381									
L217	L218	V223	E224	T227	S228	V229	K232	I235	C236	A238	L239	I240	D241	R242	P243	N244	T245	L246	F249	D250	V253	Q254	E255	T258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	W279	A280	Q283	V290	T291	S292	L293											
ARG	ARG	GLN	SER	GLU	LEU	GLY	PRO	LEU	ILE	ASP	PHE	ASN	TYR	ASN	GLN	SER	HIS	LEU	ALA	ASP	PHE	LEU	GLU	TYR	ILE	ASP	PHE	ALA	ASN	ILE	ASN	GLU	PRO	VAL	VAL	ILE	ALA	PRO	Q109	F110	S111	R112	Q113	M114	L115	D116	R117	K118	L119	L120							
M123	K126	C130	R133	E134	Y135	H136	V140	I141	K142	E146	M147	F154	L155	F156	L157	G158	G159	R160	G164	K165	Q254	I168	L173	L179	D185	S186	I187	V188	W189	L190	K191	T195	A196	P197	L203	F204	T205	D206	T207	L208	L209	M210	L211	K212	D216												

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.90Å 128.90Å 209.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8730	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0/1450	0.75	3/1950 (0.2%)
2	B	0.37	0/4101	0.66	0/5540
2	C	0.35	0/3010	0.65	1/4061 (0.0%)
All	All	0.37	0/8561	0.67	4/11551 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	N-CA-C	11.40	141.59	113.10
1	A	69	LYS	N-CA-C	6.55	128.70	111.00
1	A	68	GLY	CA-C-N	-5.44	105.24	117.20
2	C	134	GLU	CB-CA-C	5.31	121.03	110.40

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	1417	0	1365	85	0
2	B	4028	0	4052	335	0
2	C	2961	0	2998	241	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	B	31	0	12	4	0
4	C	31	0	12	3	0
5	A	32	0	0	7	0
5	B	145	0	0	22	0
5	C	83	0	0	16	0
All	All	8730	0	8439	633	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 633 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:B:302:LEU:HA	2:B:337:PHE:HZ	1.05	1.11
2:C:332:THR:HA	2:C:335:MET:HE3	1.15	1.07
2:C:433:ARG:HH11	2:C:433:ARG:HB2	1.17	1.05
2:C:307:MET:HG3	2:C:308:PRO:HD2	1.36	1.04
2:B:49:THR:HG22	2:B:52:GLU:H	1.22	1.01

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	169/204 (83%)	144 (85%)	18 (11%)	7 (4%)	3	4
2	B	493/549 (90%)	430 (87%)	46 (9%)	17 (3%)	4	6
2	C	367/549 (67%)	315 (86%)	36 (10%)	16 (4%)	3	3
All	All	1029/1302 (79%)	889 (86%)	100 (10%)	40 (4%)	3	4

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	470	ALA
2	C	342	PRO
2	C	343	LYS
2	C	450	PRO
2	C	470	ALA

5.3.2 Protein sidechains ⓘ

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	151/179 (84%)	142 (94%)	9 (6%)	22	44
2	B	457/501 (91%)	415 (91%)	42 (9%)	11	20
2	C	338/501 (68%)	312 (92%)	26 (8%)	15	29
All	All	946/1181 (80%)	869 (92%)	77 (8%)	14	26

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	365	CYS
2	B	457	ASP
2	C	433	ARG
2	B	391	SER
2	B	426	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	237	ASN
2	B	352	ASN
2	C	482	GLN
2	B	244	ASN
2	B	262	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ATP	B	551	3	27,33,33	2.51	6 (22%)	25,52,52	1.81	9 (36%)
4	ATP	C	551	3	27,33,33	1.68	6 (22%)	25,52,52	1.48	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	551	3	-	0/18/38/38	0/3/3/3
4	ATP	C	551	3	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	551	ATP	C2-N1	2.22	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	551	ATP	C2-N1	2.39	1.38	1.33
4	C	551	ATP	O4'-C4'	2.66	1.51	1.45
4	C	551	ATP	C8-N7	2.81	1.39	1.34
4	C	551	ATP	O3'-C3'	2.88	1.49	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	551	ATP	C4'-O4'-C1'	-3.09	106.47	109.77
4	B	551	ATP	C2'-C3'-C4'	-3.05	96.68	102.62
4	B	551	ATP	O4'-C4'-C3'	-2.70	99.81	105.17
4	C	551	ATP	O2'-C2'-C1'	-2.38	104.17	111.61
4	C	551	ATP	C5'-C4'-C3'	-2.29	106.55	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	551	ATP	4	0
4	C	551	ATP	3	0

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.