Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 05:38 AM EDT

PDB ID	:	1TY4
Title	:	Crystal structure of a CED-9/EGL-1 complex
Authors	:	Yan, N.; Gu, L.; Kokel, D.; Xue, D.; Shi, Y.
Deposited on	:	2004-07-07
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i)) were used in the production of this report:

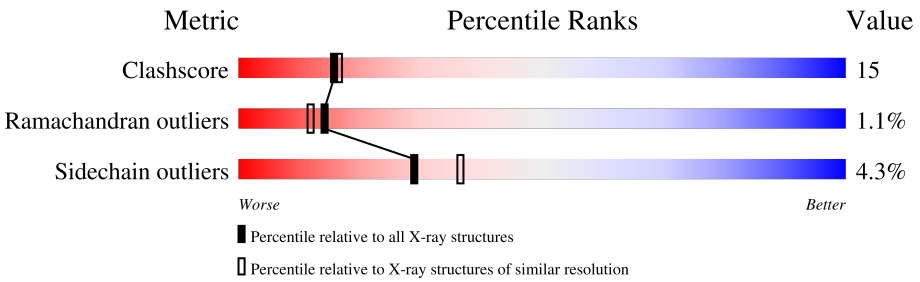
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	170	72% 22%
1	B	170	74% 22%
2	C	57	33% 16% 49%
2	D	57	33% 14% 53%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3136 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
			Total	C	N	O	S	Se			
1	A	164	1322	841	231	238	3	9	0	0	0
1	B	166	1341	851	233	246	2	9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	115	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	116	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	119	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	148	PRO	LEU	CONFLICT	UNP P41958
A	166	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	185	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	186	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	225	MSE	MET	MODIFIED RESIDUE	UNP P41958
A	231	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	97	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	115	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	116	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	119	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	148	PRO	LEU	CONFLICT	UNP P41958
B	166	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	185	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	186	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	225	MSE	MET	MODIFIED RESIDUE	UNP P41958
B	231	MSE	MET	MODIFIED RESIDUE	UNP P41958

- Molecule 2 is a protein called EGg Laying defective EGL-1, programmed cell death activator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	C	29	208	128	31	45	1	3	0	0	0
2	D	27	198	122	29	43	1	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	61	MSE	MET	MODIFIED RESIDUE	UNP O61667
C	69	MSE	MET	MODIFIED RESIDUE	UNP O61667
C	70	MSE	MET	MODIFIED RESIDUE	UNP O61667
D	61	MSE	MET	MODIFIED RESIDUE	UNP O61667
D	69	MSE	MET	MODIFIED RESIDUE	UNP O61667
D	70	MSE	MET	MODIFIED RESIDUE	UNP O61667

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	30	30	30	0	0
3	B	30	30	30	0	0
3	C	3	3	3	0	0
3	D	4	4	4	0	0

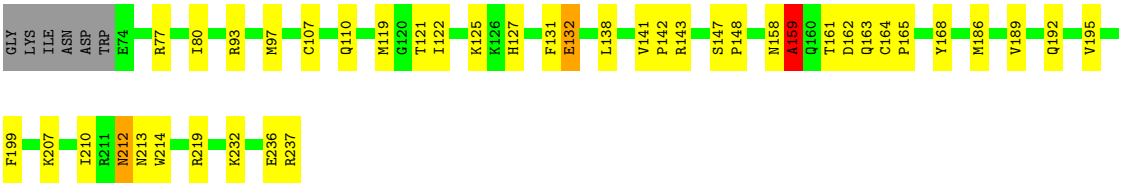
3 Residue-property plots (i)

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.

Note EDS was not executed.

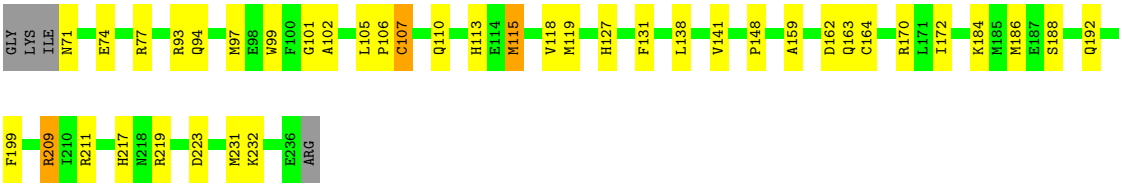
• Molecule 1: Apoptosis regulator ced-9

Chain A:



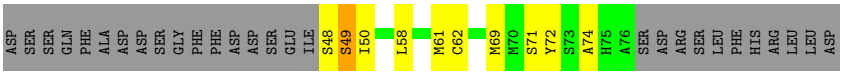
• Molecule 1: Apoptosis regulator ced-9

Chain B:



• Molecule 2: EGg Laying defective EGL-1, programmed cell death activator

Chain C:



• Molecule 2: EGg Laying defective EGL-1, programmed cell death activator

Chain D:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	93.71Å 93.71Å 57.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3136	wwPDB-VP
Average B, all atoms ($Å^2$)	44.0	wwPDB-VP

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	0.98	2/1346 (0.1%)	0.60	2/1799 (0.1%)
1	B	0.72	1/1366 (0.1%)	0.54	0/1828
2	C	1.67	1/207 (0.5%)	0.60	0/271
2	D	1.80	1/197 (0.5%)	0.75	1/257 (0.4%)
All	All	1.02	5/3116 (0.2%)	0.59	3/4155 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	62	CYS	CB-SG	-23.73	1.42	1.82
1	A	164	CYS	CB-SG	-23.69	1.42	1.82
1	A	107	CYS	CB-SG	-23.48	1.42	1.82
1	B	164	CYS	CB-SG	-23.46	1.42	1.82
2	C	62	CYS	CB-SG	-23.39	1.42	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	ASN	N-CA-C	-7.31	91.27	111.00
1	A	159	ALA	N-CA-C	-5.89	95.08	111.00
2	D	49	SER	CB-CA-C	5.76	121.04	110.10

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	1322	0	1263	38	0
1	B	1341	0	1273	39	0
2	C	208	0	188	17	0
2	D	198	0	181	12	0
3	A	30	0	0	0	0
3	B	30	0	0	1	0
3	C	3	0	0	0	0
3	D	4	0	0	1	0
All	All	3136	0	2905	88	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 15.

All (88) 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:A:186:MSE:HE3	1:A:195:VAL:HG21	1.30	1.11
1:A:161:THR:HG22	1:A:163:GLN:H	1.28	0.95
1:B:115:MSE:HE3	1:B:115:MSE:HA	1.51	0.93
1:B:209:ARG:HH21	1:B:209:ARG:CG	1.92	0.82
1:A:186:MSE:HE3	1:A:195:VAL:CG2	2.09	0.82
1:A:186:MSE:HA	1:A:186:MSE:HE2	1.61	0.81
1:A:168:TYR:HB2	2:C:69:MSE:HE1	1.66	0.78
1:A:168:TYR:HB2	2:C:69:MSE:CE	2.15	0.77
1:B:115:MSE:HE2	1:B:118:VAL:HB	1.67	0.76
2:C:48:SER:C	2:C:50:ILE:H	1.87	0.75
1:A:161:THR:HG22	1:A:163:GLN:N	2.02	0.73
1:A:158:ASN:C	1:A:159:ALA:O	2.24	0.73
1:B:106:PRO:O	2:C:74:ALA:CB	2.38	0.72
1:B:115:MSE:HA	1:B:115:MSE:CE	2.19	0.70
1:B:231:MSE:HE1	2:D:65:PHE:CZ	2.27	0.70
1:B:106:PRO:O	2:C:74:ALA:HB1	1.92	0.69
1:A:80:ILE:HD11	1:A:210:ILE:HD12	1.74	0.68
1:B:209:ARG:HH21	1:B:209:ARG:HG2	1.58	0.68
1:A:93:ARG:HA	1:A:97:MSE:O	1.95	0.66
1:B:186:MSE:HE3	1:B:192:GLN:CG	2.26	0.65
1:A:127:HIS:CG	2:C:61:MSE:HE3	2.30	0.65
1:B:186:MSE:HE3	1:B:192:GLN:HG2	1.77	0.65
1:B:131:PHE:HE1	2:D:61:MSE:HE1	1.63	0.63
1:B:127:HIS:CD2	2:D:61:MSE:HE3	2.35	0.62
2:D:65:PHE:HD2	2:D:69:MSE:HE2	1.64	0.61
2:C:72:TYR:C	2:C:74:ALA:H	2.02	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:TRP:CE3	1:B:102:ALA:HB2	2.36	0.60
1:B:209:ARG:HH21	1:B:209:ARG:HG3	1.67	0.59
1:B:159:ALA:O	1:B:170:ARG:NH2	2.35	0.59
1:A:119:MSE:HE2	1:A:119:MSE:HA	1.85	0.58
1:A:189:VAL:HA	1:A:192:GLN:HG3	1.85	0.58
2:C:71:SER:O	2:C:74:ALA:HB3	2.04	0.57
1:B:99:TRP:CD2	1:B:102:ALA:HB2	2.40	0.56
1:A:127:HIS:CD2	2:C:61:MSE:HE3	2.42	0.55
1:B:106:PRO:O	2:C:74:ALA:HB2	2.06	0.55
1:A:186:MSE:CE	1:A:195:VAL:HG21	2.20	0.55
1:B:119:MSE:HA	1:B:119:MSE:HE2	1.90	0.53
1:A:119:MSE:HE2	1:A:122:ILE:HD12	1.91	0.53
1:A:168:TYR:CB	2:C:69:MSE:HE1	2.38	0.53
1:A:77:ARG:HD2	1:A:110:GLN:OE1	2.10	0.52
1:A:165:PRO:HD2	1:A:213:ASN:OD1	2.10	0.52
1:A:131:PHE:HE1	2:C:61:MSE:HE1	1.73	0.52
2:C:48:SER:C	2:C:50:ILE:N	2.57	0.52
1:B:219:ARG:HG2	1:B:219:ARG:HH11	1.76	0.51
1:B:71:ASN:HB2	1:B:74:GLU:OE1	2.12	0.50
2:D:72:TYR:O	2:D:74:ALA:N	2.44	0.50
1:A:186:MSE:HE2	1:A:192:GLN:HG2	1.93	0.50
1:B:209:ARG:CG	1:B:209:ARG:NH2	2.62	0.50
1:B:231:MSE:HG3	2:D:72:TYR:CE1	2.47	0.50
1:A:80:ILE:CD1	1:A:210:ILE:HD12	2.42	0.49
1:A:141:VAL:HG11	1:A:148:PRO:HG2	1.94	0.49
1:A:147:SER:OG	1:A:148:PRO:HD3	2.13	0.49
1:B:127:HIS:CG	2:D:61:MSE:HE3	2.48	0.48
1:A:161:THR:HG22	1:A:162:ASP:N	2.28	0.48
2:C:48:SER:O	2:C:49:SER:HB3	2.13	0.48
2:D:65:PHE:CD2	2:D:69:MSE:HE2	2.47	0.48
1:A:161:THR:CG2	1:A:162:ASP:N	2.77	0.47
1:A:158:ASN:O	1:A:159:ALA:C	2.49	0.46
1:A:186:MSE:CE	1:A:192:GLN:HA	2.46	0.46
1:A:168:TYR:HB2	2:C:69:MSE:HE3	1.94	0.46
1:A:80:ILE:HB	1:A:207:LYS:HG3	1.98	0.46
1:B:105:LEU:C	1:B:107:CYS:H	2.19	0.46
1:A:119:MSE:CE	1:A:122:ILE:HD12	2.45	0.45
1:A:186:MSE:HA	1:A:186:MSE:CE	2.40	0.45
1:A:232:LYS:O	1:A:236:GLU:HG3	2.16	0.45
1:A:158:ASN:O	1:A:159:ALA:O	2.35	0.45
1:B:93:ARG:HA	1:B:97:MSE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ILE:HD12	2:D:69:MSE:CE	2.47	0.44
1:B:141:VAL:HG11	1:B:148:PRO:HG3	2.00	0.44
2:C:48:SER:OG	2:C:49:SER:N	2.51	0.44
1:B:163:GLN:HB2	3:B:247:HOH:O	2.19	0.43
1:A:121:THR:HG22	1:A:125:LYS:HE3	2.00	0.43
1:B:110:GLN:H	1:B:113:HIS:CD2	2.36	0.43
1:B:172:ILE:HD12	2:D:69:MSE:HE1	1.99	0.43
1:B:115:MSE:CE	1:B:118:VAL:HB	2.42	0.43
1:B:217:HIS:O	1:B:219:ARG:HG2	2.18	0.43
2:C:48:SER:O	2:C:50:ILE:N	2.52	0.43
1:B:188:SER:O	1:B:192:GLN:HG3	2.18	0.42
2:D:50:ILE:HB	3:D:16:HOH:O	2.19	0.42
1:B:115:MSE:HE1	1:B:232:LYS:HD2	2.01	0.42
1:B:219:ARG:NH2	1:B:223:ASP:OD2	2.52	0.41
1:B:105:LEU:O	1:B:107:CYS:N	2.50	0.41
1:A:142:PRO:O	1:A:143:ARG:HB2	2.21	0.41
1:A:168:TYR:H	1:A:219:ARG:NH1	2.19	0.41
1:B:131:PHE:CE1	2:D:61:MSE:HE1	2.49	0.41
1:B:184:LYS:HA	1:B:184:LYS:HD3	1.91	0.41
1:A:132:GLU:OE1	1:A:132:GLU:HA	2.21	0.41
1:B:77:ARG:HD2	1:B:110:GLN:OE1	2.21	0.41

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	162/170 (95%)	155 (96%)	5 (3%)	2 (1%)	13 10
1	B	164/170 (96%)	155 (94%)	7 (4%)	2 (1%)	13 10
2	C	27/57 (47%)	24 (89%)	3 (11%)	0	100 100
2	D	25/57 (44%)	22 (88%)	3 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	378/454 (83%)	356 (94%)	18 (5%)	4 (1%)	14 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	B	101	GLY
1	B	107	CYS
1	A	159	ALA

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	139/141 (99%)	134 (96%)	5 (4%)	35 45
1	B	142/141 (101%)	135 (95%)	7 (5%)	25 31
2	C	21/45 (47%)	19 (90%)	2 (10%)	8 8
2	D	21/45 (47%)	21 (100%)	0	100 100
All	All	323/372 (87%)	309 (96%)	14 (4%)	29 36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	GLU
1	A	138	LEU
1	A	199	PHE
1	A	214	TRP
1	A	237	ARG
1	B	94	GLN
1	B	115	MSE
1	B	138	LEU
1	B	162	ASP
1	B	199	PHE
1	B	209	ARG

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Mol	Chain	Res	Type
1	B	211	ARG
2	C	49	SER
2	C	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	113	HIS
1	A	127	HIS
1	B	90	HIS
1	B	113	HIS
1	B	163	GLN
1	B	194	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)

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.