



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:11 am BST

PDB ID : 1DEV
Title : CRYSTAL STRUCTURE OF SMAD2 MH2 DOMAIN BOUND TO THE
SMAD-BINDING DOMAIN OF SARA
Authors : Shi, Y.; Wu, G.
Deposited on : 1999-11-15
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (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) : 2.11

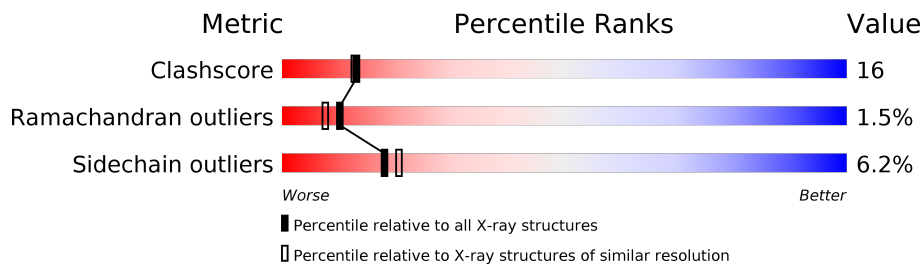
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 on 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	196	
1	C	196	
2	B	41	
2	D	41	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3643 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 MAD (mothers against decapentaplegic, Drosophila) homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1549	983	271	283	12	0	0	0
1	C	192	1528	970	266	280	12	0	0	0

- Molecule 2 is a protein called Smad anchor for receptor activation.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	41	289	179	48	60	2	0	0	0
2	D	39	277	172	46	57	2	0	0	0

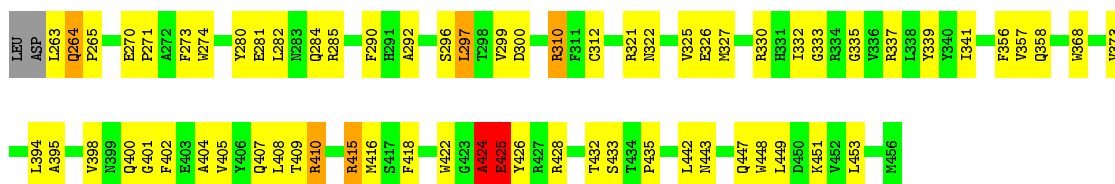
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

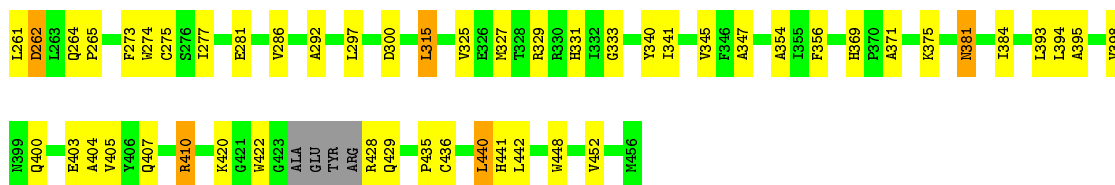
- Molecule 1: MAD (mothers against decapentaplegic, Drosophila) homolog 2

Chain A: 



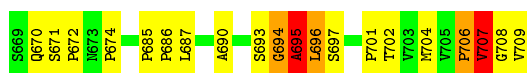
- Molecule 1: MAD (mothers against decapentaplegic, Drosophila) homolog 2

Chain C: 



- Molecule 2: Smad anchor for receptor activation

Chain B: 



- Molecule 2: Smad anchor for receptor activation

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.50Å 138.50Å 55.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.1 (20.00-2.20)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3643	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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	0.58	1/1590 (0.1%)	0.67	2/2162 (0.1%)
1	C	0.38	0/1567	0.61	0/2130
2	B	1.53	1/298 (0.3%)	1.14	3/413 (0.7%)
2	D	0.33	0/286	0.64	0/398
All	All	0.63	2/3741 (0.1%)	0.69	5/5103 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	696	LEU	N-CA	25.58	1.97	1.46
1	A	425	GLU	N-CA	17.91	1.82	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	695	ALA	C-N-CA	-14.82	84.65	121.70
1	A	424	ALA	C-N-CA	-11.74	92.36	121.70
2	B	696	LEU	N-CA-CB	-7.67	95.06	110.40
2	B	696	LEU	N-CA-C	6.41	128.29	111.00
1	A	425	GLU	N-CA-CB	-5.23	101.19	110.60

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	1549	0	1499	56	0
1	C	1528	0	1480	41	0
2	B	289	0	280	23	0
2	D	277	0	268	11	0
All	All	3643	0	3527	117	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 16.

All (117) 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:425:GLU:CA	1:A:425:GLU:N	1.82	1.43
2:B:696:LEU:N	2:B:696:LEU:CA	1.97	1.27
2:B:695:ALA:O	2:B:696:LEU:CA	1.93	1.15
2:B:695:ALA:O	2:B:696:LEU:HA	1.50	1.09
2:B:695:ALA:C	2:B:696:LEU:CA	2.26	1.02
1:A:424:ALA:C	1:A:425:GLU:CA	2.29	1.00
1:A:424:ALA:O	1:A:425:GLU:CA	2.21	0.88
1:A:424:ALA:O	1:A:425:GLU:HA	1.77	0.84
2:B:694:GLY:O	2:B:696:LEU:N	2.12	0.83
1:C:452:VAL:HB	2:D:705:VAL:HG11	1.62	0.80
1:A:265:PRO:HB3	2:B:704:MET:SD	2.22	0.79
1:A:264:GLN:HB2	1:A:265:PRO:HD2	1.64	0.78
1:A:321:ARG:HD2	1:A:326:GLU:HG2	1.65	0.77
2:B:708:GLY:O	2:B:709:VAL:HG22	1.85	0.76
1:C:420:LYS:HD2	1:C:428:ARG:HG3	1.70	0.74
1:C:381:ASN:HD21	2:D:689:GLN:HE22	1.36	0.72
1:C:369:HIS:HD2	1:C:371:ALA:H	1.41	0.69
1:C:281:GLU:HA	1:C:435:PRO:O	1.95	0.66
2:D:688:GLN:O	2:D:691:GLN:HG2	1.96	0.65
1:A:425:GLU:CB	1:A:425:GLU:N	2.60	0.64
2:B:696:LEU:N	2:B:696:LEU:CB	2.60	0.64
1:A:425:GLU:CG	1:A:425:GLU:N	2.62	0.63
1:A:357:VAL:HG22	1:A:416:MET:HG2	1.81	0.63
1:C:381:ASN:ND2	2:D:689:GLN:HE22	1.95	0.62
1:C:422:TRP:HA	1:C:429:GLN:HB3	1.82	0.60
2:B:671:SER:HB3	2:B:672:PRO:HD2	1.82	0.60
1:A:281:GLU:HA	1:A:435:PRO:O	2.00	0.60
1:A:300:ASP:HB2	1:A:333:GLY:O	2.02	0.59
1:A:310:ARG:HD2	1:A:312:CYS:SG	2.41	0.58
1:C:292:ALA:HB2	1:C:297:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:O	1:A:410:ARG:HG2	2.05	0.57
1:C:448:TRP:O	1:C:452:VAL:HG13	2.04	0.57
1:C:265:PRO:HG3	2:D:704:MET:SD	2.45	0.57
1:A:292:ALA:HB2	1:A:297:LEU:HD22	1.87	0.57
1:C:329:ARG:HG3	1:C:436:CYS:SG	2.45	0.57
2:B:696:LEU:N	2:B:696:LEU:HD13	2.21	0.56
1:C:394:LEU:O	1:C:398:VAL:HG13	2.07	0.55
1:A:296:SER:HB3	1:A:337:ARG:NH1	2.21	0.55
1:C:369:HIS:CD2	1:C:371:ALA:H	2.23	0.55
1:A:358:GLN:HE21	1:A:415:ARG:HH21	1.53	0.54
1:A:402:PHE:HB2	2:B:709:VAL:HG21	1.89	0.54
1:A:428:ARG:HB3	1:A:433:SER:HB2	1.90	0.53
1:A:448:TRP:CH2	2:B:701:PRO:HB2	2.43	0.53
1:C:400:GLN:HB3	1:C:404:ALA:CB	2.37	0.53
1:A:449:LEU:O	1:A:453:LEU:HD13	2.09	0.53
1:C:429:GLN:HE21	1:C:429:GLN:HA	1.74	0.53
1:C:347:ALA:HB2	1:C:384:ILE:HD13	1.91	0.53
2:B:694:GLY:O	2:B:695:ALA:C	2.47	0.52
2:B:696:LEU:N	2:B:696:LEU:CD1	2.73	0.51
1:A:358:GLN:HB2	1:A:422:TRP:CZ2	2.45	0.51
2:D:690:ALA:HB1	2:D:696:LEU:HD21	1.92	0.50
1:C:407:GLN:O	1:C:410:ARG:HG2	2.13	0.49
1:A:368:TRP:CE2	2:B:674:PRO:HG3	2.48	0.49
1:C:300:ASP:HB2	1:C:333:GLY:O	2.12	0.48
1:A:263:LEU:HB3	1:A:264:GLN:OE1	2.14	0.48
1:C:395:ALA:O	1:C:398:VAL:HG22	2.14	0.47
1:C:440:LEU:HD23	1:C:440:LEU:H	1.79	0.47
1:A:356:PHE:HE2	1:A:426:TYR:HH	1.63	0.47
1:C:403:GLU:O	1:C:407:GLN:HG2	2.15	0.47
1:A:358:GLN:HE21	1:A:415:ARG:NH2	2.12	0.47
1:A:395:ALA:O	1:A:398:VAL:HG22	2.14	0.47
1:C:341:ILE:HG21	2:D:690:ALA:CB	2.45	0.47
1:A:281:GLU:OE2	1:A:321:ARG:HG3	2.15	0.46
1:A:407:GLN:HE22	1:A:410:ARG:NH1	2.14	0.46
1:C:420:LYS:CD	1:C:428:ARG:HG3	2.42	0.46
1:A:325:VAL:HA	1:A:435:PRO:HB3	1.96	0.46
1:A:263:LEU:N	2:B:706:PRO:O	2.49	0.46
1:C:356:PHE:CE2	1:C:420:LYS:HE3	2.50	0.46
1:A:447:GLN:O	1:A:451:LYS:HG2	2.16	0.46
2:B:695:ALA:O	2:B:696:LEU:C	2.54	0.46
1:C:429:GLN:NE2	1:C:429:GLN:HA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:O	1:A:326:GLU:HG3	2.16	0.45
1:C:274:TRP:CD2	1:C:340:TYR:HB2	2.52	0.45
2:B:706:PRO:O	2:B:707:VAL:HG13	2.17	0.44
1:C:354:ALA:CB	1:C:375:LYS:HE3	2.47	0.44
2:D:690:ALA:HB1	2:D:696:LEU:CD2	2.47	0.44
1:A:401:GLY:O	1:A:405:VAL:HG23	2.17	0.44
1:A:425:GLU:CD	1:A:425:GLU:N	2.71	0.44
1:A:264:GLN:HB2	1:A:265:PRO:CD	2.41	0.43
1:A:409:THR:HB	1:A:410:ARG:HE	1.83	0.43
1:C:325:VAL:HA	1:C:435:PRO:HB3	1.99	0.43
1:C:327:MET:O	1:C:331:HIS:HD2	2.01	0.43
1:C:345:VAL:HG21	1:C:442:LEU:HD22	2.00	0.43
1:A:326:GLU:O	1:A:330:ARG:HG3	2.17	0.43
1:A:290:PHE:CE1	1:A:297:LEU:HD13	2.54	0.43
1:C:275:CYS:HA	1:C:441:HIS:O	2.19	0.43
1:C:420:LYS:HB2	1:C:420:LYS:NZ	2.34	0.43
1:C:428:ARG:HH22	2:D:674:PRO:HB2	1.84	0.43
2:D:677:PRO:HA	2:D:680:TYR:CZ	2.54	0.42
1:A:271:PRO:CG	1:A:274:TRP:HA	2.49	0.42
1:A:394:LEU:HA	1:A:408:LEU:HD11	2.02	0.42
1:C:274:TRP:CE2	1:C:340:TYR:HB2	2.55	0.42
1:A:273:PHE:HA	1:A:292:ALA:O	2.20	0.41
1:A:282:LEU:HD11	1:A:322:ASN:HD21	1.85	0.41
1:A:299:VAL:O	1:A:335:GLY:HA3	2.20	0.41
1:A:425:GLU:N	1:A:426:TYR:N	2.68	0.41
1:A:280:TYR:CE2	1:A:285:ARG:HD3	2.55	0.41
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.88	0.41
1:A:332:ILE:HG23	1:A:418:PHE:CD1	2.55	0.41
1:A:425:GLU:C	1:A:425:GLU:N	2.67	0.41
1:C:405:VAL:HG11	1:C:452:VAL:CG2	2.50	0.41
1:C:261:LEU:O	1:C:262:ASP:C	2.58	0.41
2:D:703:VAL:O	2:D:704:MET:HB2	2.20	0.41
1:A:296:SER:HB3	1:A:337:ARG:HH12	1.85	0.41
1:A:425:GLU:CD	1:A:425:GLU:H	2.23	0.41
1:A:265:PRO:HB2	2:B:702:THR:CG2	2.51	0.41
1:A:339:TYR:CE1	2:B:686:PRO:HG2	2.56	0.41
1:A:341:ILE:O	2:B:695:ALA:HB1	2.21	0.41
1:A:400:GLN:HB3	1:A:404:ALA:HB3	2.03	0.41
2:B:685:PRO:HA	2:B:686:PRO:HD3	1.96	0.41
1:C:273:PHE:HA	1:C:292:ALA:O	2.20	0.41
1:C:264:GLN:HA	1:C:265:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:690:ALA:O	2:B:693:SER:HB3	2.21	0.40
1:A:358:GLN:HB3	1:A:415:ARG:HB2	2.04	0.40
1:C:275:CYS:SG	1:C:277:ILE:HD11	2.62	0.40
1:A:443:ASN:O	1:A:447:GLN:HG3	2.22	0.40
1:C:277:ILE:HD12	1:C:277:ILE:N	2.37	0.40

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	192/196 (98%)	186 (97%)	5 (3%)	1 (0%)	29	31
1	C	188/196 (96%)	185 (98%)	2 (1%)	1 (0%)	29	31
2	B	39/41 (95%)	32 (82%)	3 (8%)	4 (10%)	0	0
2	D	37/41 (90%)	32 (86%)	4 (11%)	1 (3%)	5	2
All	All	456/474 (96%)	435 (95%)	14 (3%)	7 (2%)	10	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	695	ALA
2	B	707	VAL
1	A	424	ALA
2	B	706	PRO
1	C	262	ASP
2	D	695	ALA
2	B	694	GLY

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	169/171 (99%)	157 (93%)	12 (7%)	14	16
1	C	168/171 (98%)	162 (96%)	6 (4%)	35	45
2	B	35/35 (100%)	31 (89%)	4 (11%)	5	5
2	D	34/35 (97%)	31 (91%)	3 (9%)	10	10
All	All	406/412 (98%)	381 (94%)	25 (6%)	18	21

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	270	GLU
1	A	284	GLN
1	A	297	LEU
1	A	310	ARG
1	A	327	MET
1	A	373	VAL
1	A	410	ARG
1	A	415	ARG
1	A	425	GLU
1	A	432	THR
1	A	442	LEU
2	B	670	GLN
2	B	687	LEU
2	B	697	SER
2	B	707	VAL
1	C	286	VAL
1	C	315	LEU
1	C	381	ASN
1	C	393	LEU
1	C	410	ARG
1	C	440	LEU
2	D	683	THR
2	D	686	PRO
2	D	687	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	A	318	ASN
1	A	358	GLN
1	A	399	ASN
1	A	407	GLN
1	A	455	GLN
1	C	331	HIS
1	C	369	HIS
1	C	381	ASN
1	C	387	ASN
1	C	429	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 carbohydrates 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.