



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:33 PM UTC

PDB ID : 9GFO / pdb_00009gfo
Title : iASPP-CTD fusion to p63 peptide
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Deposited on : 2024-08-12
Resolution : 2.40 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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

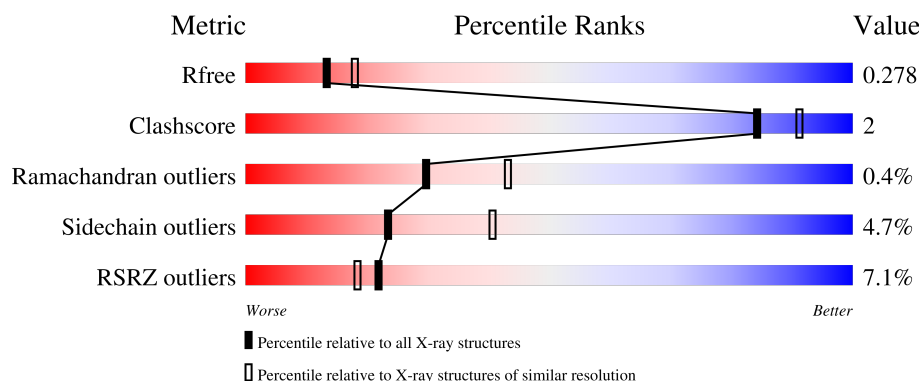
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	AAA	210	4% 90% 7% ..
1	BBB	210	11% 92% 5% ..
1	CCC	210	5% 89% 9% ..
1	DDD	210	9% 92% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6456 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 Tumor protein 63,RelA-associated inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	207	Total	C	N	O	S	0	0	0
			1592	1002	268	312	10			
1	BBB	207	Total	C	N	O	S	0	0	0
			1592	1002	268	312	10			
1	CCC	206	Total	C	N	O	S	0	0	0
			1586	999	267	310	10			
1	DDD	210	Total	C	N	O	S	0	0	0
			1613	1015	272	316	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	21	Total	O	0	0
			21	21		
2	BBB	18	Total	O	0	0
			18	18		
2	CCC	19	Total	O	0	0
			19	19		
2	DDD	15	Total	O	0	0
			15	15		

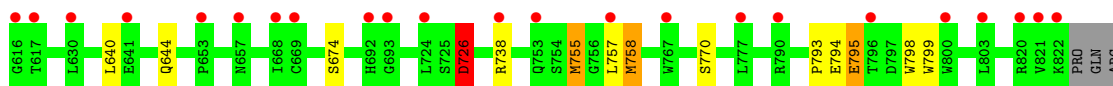
3 Residue-property plots [i](#)

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 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: Tumor protein 63,RelA-associated inhibitor



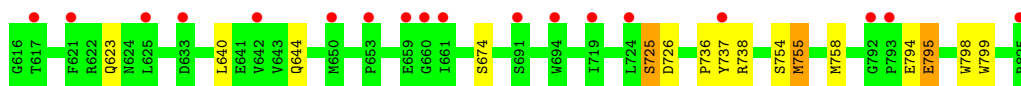
- Molecule 1: Tumor protein 63,RelA-associated inhibitor



- Molecule 1: Tumor protein 63,RelA-associated inhibitor



- Molecule 1: Tumor protein 63,RelA-associated inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.12Å 94.12Å 179.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.40 47.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.24-2.40) 99.9 (47.24-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.243 , 0.280 0.243 , 0.278	Depositor DCC
R_{free} test set	2550 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6456	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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

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	AAA	1.04	0/1632	1.38	0/2227
1	BBB	1.03	0/1632	1.40	0/2227
1	CCC	1.07	0/1626	1.41	2/2219 (0.1%)
1	DDD	1.04	0/1654	1.41	0/2258
All	All	1.04	0/6544	1.40	2/8931 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	CCC	815	PHE	CA-C-N	5.28	126.12	121.58
1	CCC	815	PHE	C-N-CA	5.28	126.12	121.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	617	THR	Peptide

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	AAA	1592	0	1495	7	0
1	BBB	1592	0	1495	8	0
1	CCC	1586	0	1487	8	0
1	DDD	1613	0	1512	8	0
2	AAA	21	0	0	0	0
2	BBB	18	0	0	1	0
2	CCC	19	0	0	3	0
2	DDD	15	0	0	0	0
All	All	6456	0	5989	29	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 2.

All (29) 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:CCC:633:ASP:HB2	2:CCC:911:HOH:O	1.54	1.05
1:CCC:750:ASP:HB3	2:CCC:915:HOH:O	1.79	0.81
1:CCC:655:GLN:HG2	2:CCC:917:HOH:O	2.01	0.60
1:BBB:795:GLU:HG2	1:BBB:798:TRP:CD1	2.41	0.56
1:BBB:758:MET:HG2	1:DDD:736:PRO:O	2.09	0.52
1:DDD:725:SER:O	1:DDD:726:ASP:CG	2.52	0.51
1:CCC:755:MET:HG2	1:CCC:799:TRP:HH2	1.76	0.51
1:BBB:758:MET:HA	1:DDD:737:TYR:HD1	1.75	0.50
1:CCC:640:LEU:O	1:CCC:644:GLN:HG3	2.12	0.50
1:BBB:640:LEU:O	1:BBB:644:GLN:HG3	2.12	0.49
1:DDD:640:LEU:O	1:DDD:644:GLN:HG3	2.12	0.49
1:DDD:795:GLU:HG2	1:DDD:798:TRP:CD1	2.47	0.49
1:AAA:640:LEU:O	1:AAA:644:GLN:HG3	2.12	0.48
1:AAA:726:ASP:C	1:AAA:726:ASP:OD1	2.57	0.47
1:BBB:726:ASP:OD1	1:BBB:726:ASP:C	2.57	0.47
1:DDD:726:ASP:OD1	1:DDD:726:ASP:C	2.58	0.46
1:CCC:736:PRO:HA	1:CCC:741:TYR:CG	2.53	0.43
1:DDD:755:MET:HG2	1:DDD:799:TRP:HH2	1.83	0.43
1:BBB:793:PRO:HD3	2:BBB:909:HOH:O	2.19	0.42
1:BBB:757:LEU:HD12	1:BBB:757:LEU:HA	1.87	0.42
1:AAA:795:GLU:HG2	1:AAA:798:TRP:CD1	2.55	0.42
1:AAA:811:PRO:HG2	1:AAA:814:TYR:CD1	2.55	0.42
1:DDD:754:SER:HB2	1:DDD:758:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:755:MET:HG2	1:AAA:799:TRP:HH2	1.86	0.41
1:CCC:755:MET:HE1	1:CCC:815:PHE:O	2.19	0.41
1:BBB:755:MET:HG2	1:BBB:799:TRP:HH2	1.86	0.41
1:AAA:736:PRO:HA	1:AAA:741:TYR:CG	2.56	0.41
1:CCC:643:VAL:O	1:CCC:647:VAL:HG23	2.21	0.40
1:AAA:799:TRP:O	1:AAA:809:TYR:HA	2.21	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	AAA	205/210 (98%)	195 (95%)	9 (4%)	1 (0%)	24	37
1	BBB	205/210 (98%)	196 (96%)	8 (4%)	1 (0%)	24	37
1	CCC	204/210 (97%)	194 (95%)	9 (4%)	1 (0%)	24	37
1	DDD	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
All	All	822/840 (98%)	781 (95%)	38 (5%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	726	ASP
1	BBB	726	ASP
1	CCC	792	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	AAA	166/169 (98%)	158 (95%)	8 (5%)	23	40
1	BBB	166/169 (98%)	158 (95%)	8 (5%)	23	40
1	CCC	165/169 (98%)	157 (95%)	8 (5%)	23	40
1	DDD	168/169 (99%)	161 (96%)	7 (4%)	26	45
All	All	665/676 (98%)	634 (95%)	31 (5%)	23	41

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	618	LYS
1	AAA	623	GLN
1	AAA	674	SER
1	AAA	726	ASP
1	AAA	738	ARG
1	AAA	755	MET
1	AAA	770	SER
1	AAA	795	GLU
1	BBB	674	SER
1	BBB	726	ASP
1	BBB	738	ARG
1	BBB	755	MET
1	BBB	758	MET
1	BBB	770	SER
1	BBB	794	GLU
1	BBB	795	GLU
1	CCC	623	GLN
1	CCC	674	SER
1	CCC	724	LEU
1	CCC	738	ARG
1	CCC	755	MET
1	CCC	770	SER
1	CCC	790	ARG
1	CCC	795	GLU
1	DDD	623	GLN
1	DDD	674	SER
1	DDD	725	SER
1	DDD	738	ARG
1	DDD	755	MET
1	DDD	794	GLU

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Mol	Chain	Res	Type
1	DDD	795	GLU

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 oligosaccharides 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

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	AAA	207/210 (98%)	0.36	8 (3%) 43 39	44, 62, 110, 132	0
1	BBB	207/210 (98%)	0.92	23 (11%) 10 7	50, 75, 119, 171	0
1	CCC	206/210 (98%)	0.51	10 (4%) 35 31	43, 66, 113, 145	0
1	DDD	210/210 (100%)	0.73	18 (8%) 16 13	44, 80, 133, 157	0
All	All	830/840 (98%)	0.63	59 (7%) 22 18	43, 70, 124, 171	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	653	PRO	5.2
1	CCC	759	ASN	4.8
1	DDD	621	PHE	4.7
1	BBB	653	PRO	4.7
1	DDD	825	ARG	4.5
1	AAA	653	PRO	4.1
1	CCC	617	THR	4.1
1	DDD	792	GLY	4.0
1	BBB	617	THR	3.7
1	BBB	821	VAL	3.5
1	BBB	616	GLY	3.5
1	AAA	621	PHE	3.5
1	AAA	822	LYS	3.3
1	CCC	822	LYS	3.2
1	BBB	822	LYS	3.1
1	BBB	767	TRP	3.1
1	DDD	653	PRO	3.1
1	DDD	724	LEU	3.0
1	BBB	757	LEU	3.0
1	CCC	789	ARG	2.8
1	BBB	803	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	BBB	820	ARG	2.7
1	BBB	669	CYS	2.7
1	AAA	617	THR	2.7
1	CCC	793	PRO	2.6
1	BBB	693	GLY	2.6
1	AAA	630	LEU	2.6
1	CCC	817	LEU	2.5
1	BBB	796	THR	2.5
1	CCC	794	GLU	2.4
1	BBB	777	LEU	2.4
1	BBB	641	GLU	2.4
1	BBB	668	ILE	2.4
1	DDD	793	PRO	2.4
1	CCC	724	LEU	2.4
1	BBB	753	GLN	2.4
1	AAA	669	CYS	2.4
1	DDD	617	THR	2.3
1	DDD	660	GLY	2.3
1	DDD	737	TYR	2.3
1	BBB	790	ARG	2.2
1	DDD	642	VAL	2.2
1	DDD	661	ILE	2.2
1	BBB	800	TRP	2.2
1	AAA	793	PRO	2.2
1	BBB	657	ASN	2.1
1	CCC	757	LEU	2.1
1	DDD	625	LEU	2.1
1	DDD	719	ILE	2.1
1	DDD	659	GLU	2.1
1	BBB	630	LEU	2.1
1	DDD	650	MET	2.1
1	BBB	738	ARG	2.1
1	AAA	661	ILE	2.1
1	BBB	692	HIS	2.1
1	BBB	724	LEU	2.1
1	DDD	694	TRP	2.1
1	DDD	633	ASP	2.1
1	DDD	691	SER	2.0

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 oligosaccharides 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.