

Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 05:33 am BST

PDB ID	:	4CGW
Title	:	Second TPR of Spaghetti (RPAP3) bound to HSP90 peptide SRMEEVD
Authors	:	Roe, S.M.; Pal, M.
Deposited on		
Resolution	:	3.00 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 (1)) were used in the production of this report:

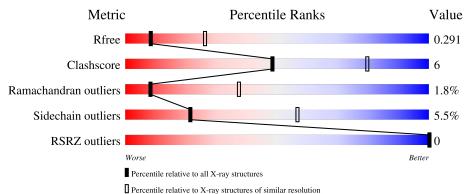
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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% 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	А	117	75%	21% ••
1	В	117	81%	11% 8%
2	С	7	71%	29%
2	D	7	29% 43%	29%



$4 \mathrm{CGW}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1798 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 RNA POLYMERASE II-ASSOCIATED PROTEIN 3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	115	Total	С	Ν	0	S	0	0	0
	A	115	872	547	155	167	3	0	0	0
1	В	108	Total	С	Ν	Ο	S	0	0	Ο
	D	108	823	516	145	159	3	0	0	0

• Molecule 2 is a protein called HEAT SHOCK PROTEIN HSP 90-ALPHA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	7	Total C N O S 52 30 7 14 1	0	0	0
2	D	5	Total C N O 39 22 5 12	0	0	0

• Molecule 3 is water.

Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	8	Total O 8 8	0	0
3	В	4	Total O 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 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: RNA POLYMERASE II-ASSOCIATED PROTEIN 3

Chain A:	75%	21% ••
SER THR E267 Q276 Q277 N277 X279 S2 <u>84</u>	7292 7292 7298 7298 7298 7298 0312 6313 7314 7314 7314 7314 7315 7326 7326 7326 7326 7326 7326 7326 7326	Y349 S350 R355 R355 R355 R355 E360 E366 E366 E366 E365 E374 E374
• Molecule 1:	RNA POLYMERASE II-ASSOC	IATED PROTEIN 3
Chain B:	81%	11% 8%
SER THR GLU GLV GLV GLV CLN GLN	q280 q281 A281 A282 A281 A281 A281 A281 A281 A281 A316 L316 L316 L316 L316 L316 L316 L316 L316 L316 L316 L3179 R360 R360 R360 R360 R360 R360 R360 R379 R379 R379 R360 R379 R379 R379 R379 R379 R379 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 R370 	
• Molecule 2:	HEAT SHOCK PROTEIN HSP	90-ALPHA
Chain C:	71%	29%
81 M3 H2 H2 H2 H2 H2 H2 H2 H2 H2 H2 H2 H2 H2		
• Molecule 2:	HEAT SHOCK PROTEIN HSP	90-ALPHA
Chain D:	29% 43%	29%
SER ARG E5 D7 D7		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	63.57Å 96.51Å 52.09Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 - 3.00	Depositor
Resolution (A)	48.25 - 3.00	EDS
% Data completeness	93.2 (48.26-3.00)	Depositor
(in resolution range)	86.8 (48.25-3.00)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.76 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.241 , 0.291	Depositor
R, R_{free}	0.241 , 0.291	DCC
R_{free} test set	294 reflections $(4.63%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	55.5	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30, 31.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1798	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Mol Chain		lengths	Bond angles	
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.23	0/883	0.38	0/1184
1	В	0.24	0/833	0.39	0/1118
2	С	0.21	0/51	0.43	0/66
2	D	0.25	0/38	0.43	0/49
All	All	0.23	0/1805	0.39	0/2417

There are no bond length outliers.

There are no bond angle outliers.

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	А	872	0	842	13	0
1	В	823	0	788	6	0
2	С	52	0	40	0	0
2	D	39	0	26	4	0
3	А	8	0	0	0	0
3	В	4	0	0	1	0
All	All	1798	0	1696	21	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 6.

All (21) 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:B:290:ASN:ND2	2:D:7:ASP:OD2	2.20	0.73
1:A:365:LYS:HB3	1:A:368:GLU:HG3	1.77	0.66
1:A:324:MET:HE1	1:A:355:ARG:HG2	1.81	0.63
1:B:316:ALA:HB2	1:B:345:LEU:HB2	1.84	0.59
1:A:312:ASP:OD1	1:A:314:ALA:N	2.38	0.52
1:A:360:ARG:HB3	1:A:365:LYS:HB2	1.91	0.52
1:A:371:GLN:HA	1:A:374:GLU:HG2	1.91	0.51
1:A:276:GLN:O	1:A:279:LYS:N	2.42	0.48
1:B:282:ALA:HB1	1:B:318:LEU:HD21	1.95	0.48
1:B:360:ARG:HB3	1:B:365:LYS:HB2	1.97	0.46
3:B:2003:HOH:O	2:D:3:MET:O	2.20	0.46
1:B:317:LEU:HD11	2:D:7:ASP:HA	1.98	0.45
1:A:360:ARG:HD3	1:A:368:GLU:HB2	1.99	0.44
1:A:312:ASP:HA	1:A:313:GLY:HA3	1.52	0.43
1:A:298:TYR:O	1:A:302:ILE:HG13	2.18	0.43
1:B:298:TYR:CZ	1:B:328:LYS:HD3	2.54	0.42
1:A:339:CYS:HB3	1:A:356:ARG:HB2	2.02	0.42
1:A:292:PHE:HB3	1:A:297:LYS:O	2.20	0.41
1:A:318:LEU:HB2	1:A:319:PRO:HD3	2.02	0.41
2:D:5:GLU:H	2:D:5:GLU:HG3	1.71	0.41
1:A:326:TYR:CD1	1:A:331:LYS:HG3	2.56	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	А	113/117~(97%)	106 (94%)	4 (4%)	3~(3%)	5 26	
1	В	106/117~(91%)	102 (96%)	3~(3%)	1 (1%)	17 55	
2	С	5/7~(71%)	5 (100%)	0	0	100 100	
2	D	3/7~(43%)	3~(100%)	0	0	100 100	
All	All	227/248~(92%)	216 (95%)	7(3%)	4 (2%)	8 37	





All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	277	GLN
1	А	276	GLN
1	А	312	ASP
1	В	379	LEU

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	А	80/92~(87%)	75~(94%)	5~(6%)	18 51
1	В	75/92~(82%)	73~(97%)	2(3%)	44 77
2	С	5/7~(71%)	3~(60%)	2 (40%)	0 0
2	D	4/7~(57%)	4 (100%)	0	100 100
All	All	164/198~(83%)	155~(94%)	9~(6%)	21 57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	284	SER
1	А	328	LYS
1	А	349	TYR
1	А	350	SER
1	А	368	GLU
1	В	280	GLN
1	В	349	TYR
2	С	3	MET
2	С	4	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 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)

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		RZ>2	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	115/117~(98%)	-0.19	0	100	100	48, 58, 86, 100	0
1	В	108/117~(92%)	-0.30	0	100	100	50, 60, 85, 113	0
2	С	7/7~(100%)	-0.06	0	100	100	63, 64, 79, 82	0
2	D	5/7~(71%)	-0.02	0	100	100	74, 77, 89, 89	0
All	All	235/248~(94%)	-0.24	0	100	100	48, 59, 88, 113	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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.

