wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 03:37 PM EDT

PDB ID	:	6SWG
Title	:	Crystal structure of the TASOR-Periphilin core complex
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Deposited on	:	2019-09-20
Resolution	:	2.51 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
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:

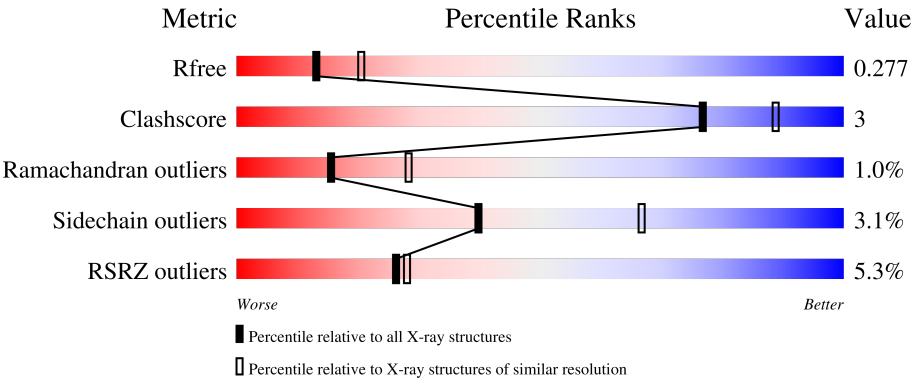
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.51 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	A	94	5% 68% 9% 23%
1	B	94	% 76% • • 21%
2	C	83	6% 63% 10% • • 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3391 atoms, of which 1702 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 Periphilin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	72	Total	C	H	N	O	S	0	0	0
			1175	367	589	100	115	4			
1	B	74	Total	C	H	N	O	S	0	0	0
			1208	377	607	102	118	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	MET	-	initiating methionine	UNP Q8NEY8
A	275	GLY	-	expression tag	UNP Q8NEY8
A	276	SER	-	expression tag	UNP Q8NEY8
A	277	SER	-	expression tag	UNP Q8NEY8
A	278	HIS	-	expression tag	UNP Q8NEY8
A	279	HIS	-	expression tag	UNP Q8NEY8
A	280	HIS	-	expression tag	UNP Q8NEY8
A	281	HIS	-	expression tag	UNP Q8NEY8
A	282	HIS	-	expression tag	UNP Q8NEY8
A	283	HIS	-	expression tag	UNP Q8NEY8
A	284	SER	-	expression tag	UNP Q8NEY8
A	285	GLN	-	expression tag	UNP Q8NEY8
A	286	GLU	-	expression tag	UNP Q8NEY8
A	287	ASN	-	expression tag	UNP Q8NEY8
A	288	LEU	-	expression tag	UNP Q8NEY8
A	289	TYR	-	expression tag	UNP Q8NEY8
A	290	PHE	-	expression tag	UNP Q8NEY8
A	291	GLN	-	expression tag	UNP Q8NEY8
B	274	MET	-	initiating methionine	UNP Q8NEY8
B	275	GLY	-	expression tag	UNP Q8NEY8
B	276	SER	-	expression tag	UNP Q8NEY8
B	277	SER	-	expression tag	UNP Q8NEY8
B	278	HIS	-	expression tag	UNP Q8NEY8
B	279	HIS	-	expression tag	UNP Q8NEY8
B	280	HIS	-	expression tag	UNP Q8NEY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	281	HIS	-	expression tag	UNP Q8NEY8
B	282	HIS	-	expression tag	UNP Q8NEY8
B	283	HIS	-	expression tag	UNP Q8NEY8
B	284	SER	-	expression tag	UNP Q8NEY8
B	285	GLN	-	expression tag	UNP Q8NEY8
B	286	GLU	-	expression tag	UNP Q8NEY8
B	287	ASN	-	expression tag	UNP Q8NEY8
B	288	LEU	-	expression tag	UNP Q8NEY8
B	289	TYR	-	expression tag	UNP Q8NEY8
B	290	PHE	-	expression tag	UNP Q8NEY8
B	291	GLN	-	expression tag	UNP Q8NEY8

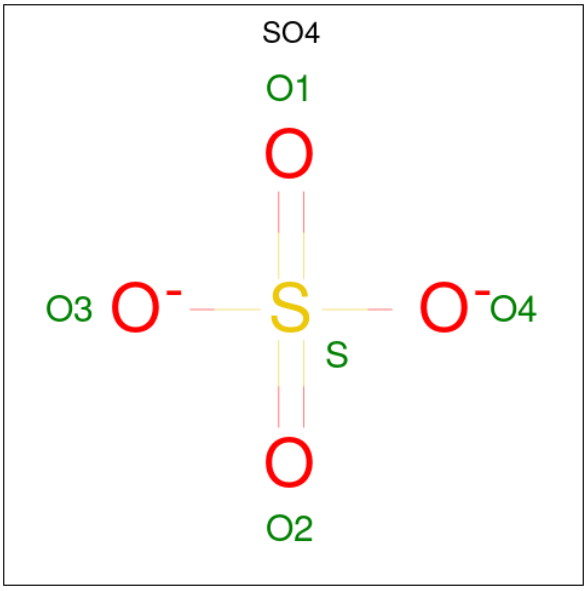
- Molecule 2 is a protein called Protein TASOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	63	Total	C	H	N	O	0	0	0
			1003	316	506	81	100			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1013	MET	-	initiating methionine	UNP Q9UK61

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

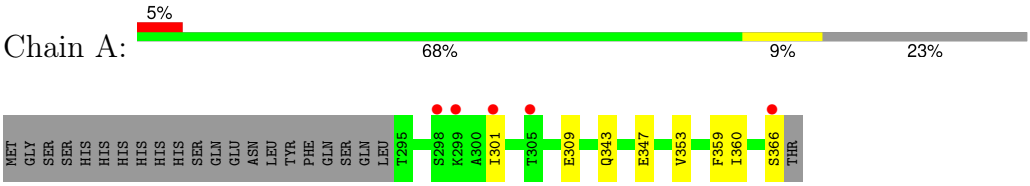


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0

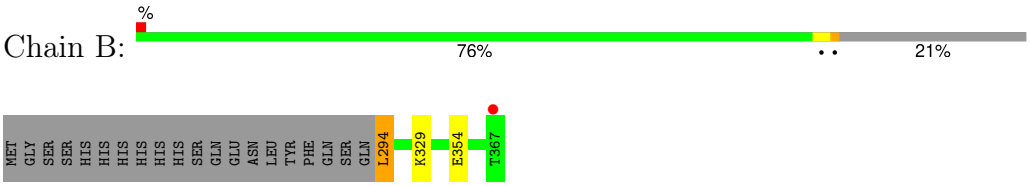
3 Residue-property plots (i)

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.

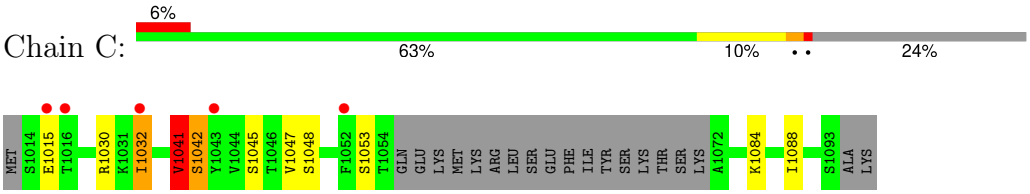
• Molecule 1: Periphilin-1



• Molecule 1: Periphilin-1



• Molecule 2: Protein TASOR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.57Å 93.57Å 84.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.98 – 2.51 40.98 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.98-2.51) 96.3 (40.98-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.228 , 0.271 0.237 , 0.277	Depositor DCC
R_{free} test set	785 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	83.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 77.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3391	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.65	0/593	0.70	0/793
1	B	0.81	0/608	0.91	1/814 (0.1%)
2	C	0.69	0/502	0.68	0/676
All	All	0.72	0/1703	0.77	1/2283 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	294	LEU	CA-CB-CG	8.58	135.04	115.30

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	586	589	589	7	0
1	B	601	607	607	2	1
2	C	497	506	506	6	1
3	C	5	0	0	0	0
All	All	1689	1702	1702	10	1

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 3.

The worst 5 of 10 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:C:1015:GLU:OE1	2:C:1015:GLU:N	2.14	0.81
1:A:347:GLU:OE1	1:B:329:LYS:NZ	2.33	0.61
1:A:353:VAL:HG22	2:C:1032:ILE:HD13	1.89	0.55
1:A:301:ILE:HD13	1:A:359:PHE:HE2	1.74	0.53
1:A:309:GLU:HB2	2:C:1047:VAL:HG21	1.92	0.51

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:OE1	2:C:1030:ARG:HH21[4_456]	1.52	0.08

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	70/94 (74%)	69 (99%)	1 (1%)	0	100 100
1	B	72/94 (77%)	71 (99%)	1 (1%)	0	100 100
2	C	59/83 (71%)	54 (92%)	3 (5%)	2 (3%)	3 5
All	All	201/271 (74%)	194 (96%)	5 (2%)	2 (1%)	15 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1041	VAL
2	C	1042	SER

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	66/87 (76%)	65 (98%)	1 (2%)	65 85
1	B	68/87 (78%)	67 (98%)	1 (2%)	65 85
2	C	58/77 (75%)	54 (93%)	4 (7%)	15 30
All	All	192/251 (76%)	186 (97%)	6 (3%)	40 67

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1041	VAL
2	C	1048	SER
2	C	1053	SER
1	B	294	LEU
1	A	366	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
3	SO4	C	1101	-	4,4,4	0.19	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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			OWAB(Å^2)	Q<0.9
1	A	72/94 (76%)	0.82	5 (6%)	16	17	76, 111, 159, 166	0
1	B	74/94 (78%)	0.58	1 (1%)	75	77	73, 91, 125, 135	0
2	C	63/83 (75%)	0.68	5 (7%)	12	12	77, 124, 178, 209	0
All	All	209/271 (77%)	0.69	11 (5%)	26	28	73, 103, 163, 209	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ILE	4.4
2	C	1043	TYR	4.3
1	B	367	THR	2.7
2	C	1052	PHE	2.7
1	A	366	SER	2.6

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

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	1101	5/5	0.90	0.17	150,150,151,153	0

6.5 Other polymers (i)

There are no such residues in this entry.