

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2J9Q
Title	:	A novel conformation for the TPR domain of pex5p
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Deposited on	:	2006-11-15
Resolution	:	2.65 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
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

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 2.65 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.



${f Metric} egin{array}{c} {f Whole archive} \ (\# { m Entries}) \end{array}$		${f Similar\ resolution}\ (\# Entries, resolution\ range(Å))$		
R _{free}	130704	1332 (2.68-2.64)		
Clashscore	141614	1374 (2.68-2.64)		
RSRZ outliers	127900	1318 (2.68-2.64)		

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 cha	in		
1	А	328	5% 79%		12%	9%
1	В	328	<u>19%</u> 62%	20%	18%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4468 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 PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	300	Total 2356	C 1482	N 409	O 452	S 13	0	1	0
1	В	269	Total 2092	C 1316	N 365	O 400	S 11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	312	GLY	-	expression tag	UNP P50542
А	313	MET	-	expression tag	UNP P50542
А	314	GLY	-	expression tag	UNP P50542
А	425	ILE	THR	conflict	UNP P50542
В	312	GLY	-	expression tag	UNP P50542
В	313	MET	-	expression tag	UNP P50542
B	314	GLY	-	expression tag	UNP P50542
В	425	ILE	THR	conflict	UNP P50542

• Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Sr 1 1	0	0
2	В	1	Total Sr 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	13	Total O 13 13	0	0
3	В	5	Total O 5 5	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: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	53.67Å 91.41Å 119.89Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	20.00 - 2.65	Depositor
	19.53 - 2.65	EDS
% Data completeness	93.8 (20.00-2.65)	Depositor
(in resolution range)	94.0(19.53-2.65)	EDS
R_{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.52 (at 2.67 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R R.	0.241 , 0.300	Depositor
n, n_{free}	0.239 , 0.294	DCC
R_{free} test set	833 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	45.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.32 , 79.9	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.95% 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)

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

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.32	0/2403	0.48	0/3256	
1	В	0.32	0/2129	0.49	0/2887	
All	All	0.32	0/4532	0.49	0/6143	

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	2356	0	2308	38	0
1	В	2092	0	2068	61	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	13	0	0	1	0
3	В	5	0	0	0	0
All	All	4468	0	4376	89	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 10.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:468:PHE:CE1	1:B:500:LEU:HD11	1.96	0.99
1:B:411:VAL:HG11	1:B:523:LEU:HD22	1.66	0.78
1:A:440:VAL:HG12	1:A:441:THR:H	1.51	0.76
1:A:609:LEU:HD23	1:B:609:LEU:HD23	1.70	0.72
1:B:392:LEU:HD13	1:B:409:LEU:HB3	1.74	0.70
1:B:409:LEU:HD12	1:B:410:ALA:N	2.07	0.70
1:A:609:LEU:HD21	1:B:606:THR:HG23	1.73	0.69
1:A:422:ALA:HB3	1:A:500:LEU:HD11	1.76	0.68
1:B:468:PHE:CD1	1:B:500:LEU:HD11	2.30	0.66
1:B:410:ALA:HB2	1:B:426:LEU:HD21	1.81	0.63
1:B:422:ALA:O	1:B:425:ILE:HG22	1.99	0.63
1:B:392:LEU:HD13	1:B:409:LEU:CB	2.30	0.60
1:B:418:LEU:O	1:B:422:ALA:HB3	2.01	0.60
1:B:520:ASN:O	1:B:551:LEU:HD13	2.02	0.59
1:A:604:TRP:CE2	1:A:626:ARG:HG3	2.37	0.59
1:B:499:ASN:HD21	1:B:534:ASN:HD22	1.50	0.59
1:B:380:ALA:HB1	1:B:412:SER:CB	2.33	0.59
1:A:316:THR:HG22	1:A:317:SER:H	1.69	0.57
1:A:567:ILE:CG2	1:B:613:MET:CE	2.83	0.57
1:A:567:ILE:HG21	1:B:613:MET:CE	2.35	0.57
1:B:576:VAL:HG13	1:B:607:LEU:HD11	1.87	0.56
1:B:500:LEU:HD12	1:B:500:LEU:C	2.26	0.56
1:B:429:TRP:HE3	1:B:430:LEU:HD12	1.71	0.55
1:B:567:ILE:HD11	1:B:610:ALA:HB2	1.87	0.55
1:B:439:LEU:HD22	1:B:440:VAL:N	2.23	0.54
1:B:410:ALA:CB	1:B:426:LEU:HD21	2.37	0.54
1:A:567:ILE:CG2	1:B:613:MET:HE2	2.38	0.53
1:B:406:LEU:HD13	1:B:429:TRP:HE1	1.72	0.53
1:B:545:TYR:CZ	1:B:561:ASN:HB3	2.44	0.53
1:A:419:GLN:NE2	3:A:2005:HOH:O	2.42	0.52
1:B:583:LEU:HD13	1:B:604:TRP:CZ2	2.44	0.52
1:A:613:MET:CE	1:B:613:MET:CE	2.88	0.52
1:B:476:LEU:HD13	1:B:494:LEU:HD11	1.91	0.52
1:A:567:ILE:HG21	1:B:613:MET:HE3	1.92	0.52
1:A:545:TYR:CZ	1:A:561:ASN:HB3	2.46	0.51
1:B:587:ARG:HG3	1:B:628:LEU:HD23	1.92	0.51
1:B:494:LEU:HD22	1:B:498:PHE:CD2	2.46	0.50
1:A:576:VAL:HG11	1:A:635:PHE:CE2	2.46	0.50
1:B:358:PHE:HB2	1:B:375:LEU:HD13	1.93	0.49
1:B:383:GLU:CD	1:B:598:ALA:HB1	2.31	0.49
1:B:409:LEU:HD12	1:B:410:ALA:HB2	1.93	0.49



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:500:LEU:HD12	1:B:501:SER:N	2.28	0.49	
1:A:428:ASP:HA	1:A:431:ARG:HG2	1.94	0.49	
1:B:499:ASN:HD21	1:B:534:ASN:ND2	2.11	0.49	
1:B:407:MET:CE	1:B:410:ALA:HB3	2.44	0.48	
1:B:542:VAL:HG13	1:B:562:LEU:HD11	1.95	0.48	
1:A:467:LEU:HD22	1:A:471:VAL:HG23	1.95	0.48	
1:B:378:THR:HG22	1:B:378:THR:O	2.14	0.47	
1:A:422:ALA:CB	1:A:500:LEU:HD11	2.44	0.47	
1:A:557:ARG:HA	1:A:599:MET:HE1	1.96	0.47	
1:A:351:LEU:N	1:A:352:PRO:CD	2.78	0.47	
1:A:316:THR:HG22	1:A:317:SER:N	2.29	0.47	
1:B:493:GLY:O	1:B:496:VAL:HG22	2.15	0.47	
1:B:358:PHE:O	1:B:362:VAL:HG13	2.14	0.46	
1:B:617:SER:HA	1:B:620:TYR:CE1	2.51	0.46	
1:A:419:GLN:HB3	1:A:500:LEU:HD22	1.98	0.46	
1:A:324:TYR:OH	1:A:375:LEU:HD11	2.16	0.45	
1:A:424:GLU:HG3	1:A:467:LEU:HD11	1.98	0.45	
1:B:380:ALA:HB1	1:B:412:SER:OG	2.17	0.44	
1:B:409:LEU:HD13	1:B:425:ILE:HG23	2.00	0.44	
1:B:437:ALA:O	1:B:439:LEU:HD12	2.19	0.43	
1:A:466:SER:OG	1:A:469:LEU:HD13	2.18	0.43	
1:A:423:CYS:HB3	1:A:471:VAL:HG21	2.01	0.43	
1:A:504:TYR:O	1:A:508:VAL:HG23	2.18	0.43	
1:A:604:TRP:CZ2	1:A:626:ARG:HG3	2.53	0.43	
1:A:586:GLN:O	1:A:590:ARG:HG3	2.18	0.43	
1:B:572:HIS:HB2	1:B:614:LEU:HD13	2.00	0.43	
1:B:354:ALA:CB	1:B:378:THR:HG21	2.49	0.42	
1:A:567:ILE:CG2	1:B:613:MET:HE3	2.48	0.42	
1:B:507:ALA:HB3	1:B:531:THR:HG21	2.02	0.42	
1:B:467:LEU:HD13	1:B:467:LEU:C	2.40	0.42	
1:B:468:PHE:CZ	1:B:501:SER:HB3	2.55	0.42	
1:A:514:ALA:CB	1:A:524:LEU:HD11	2.50	0.41	
1:A:396:LEU:HD21	1:A:406:LEU:HG	2.02	0.41	
1:B:560:TYR:CZ	1:B:564:ILE:HD11	2.55	0.41	
1:A:431:ARG:HB3	1:A:440:VAL:HG21	2.02	0.41	
1:B:609:LEU:HG	1:B:613:MET:CE	2.50	0.41	
1:A:542:VAL:HG13	1:A:562:LEU:HD11	2.03	0.41	
1:A:467:LEU:HD22	1:A:471:VAL:CG2	2.51	0.41	
1:B:407:MET:HE1	1:B:410:ALA:HB3	2.02	0.41	
1:B:438:HIS:O	1:B:438:HIS:CG	2.74	0.41	
1:A:423:CYS:HB2	1:A:467:LEU:HD13	2.03	0.41	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:613:MET:HE1	1:B:613:MET:HE2	2.04	0.40	
1:A:618:ASP:OD2	1:A:618:ASP:N	2.54	0.40	
1:B:409:LEU:HD22	1:B:425:ILE:HD12	2.02	0.40	
1:B:469:LEU:HD12	1:B:472:LYS:HE3	2.03	0.40	
1:B:437:ALA:O	1:B:439:LEU:N	2.54	0.40	
1:A:613:MET:CE	1:B:613:MET:HE2	2.51	0.40	
1:B:609:LEU:HG	1:B:613:MET:HE3	2.03	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 (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	$OWAB(Å^2)$	Q<0.9
1	А	300/328~(91%)	0.45	18 (6%) 21 18	39, 44, 47, 52	0
1	В	269/328~(82%)	1.16	63~(23%) 0 0	39, 44, 50, 57	0
All	All	569/656~(86%)	0.79	81 (14%) 2 1	39, 44, 48, 57	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	401	ASP	8.7
1	В	594	GLY	8.1
1	В	591	GLY	7.9
1	В	403	GLN	6.6
1	В	415	ASN	6.4
1	А	441	THR	6.4
1	В	354	ALA	6.1
1	В	405	ALA	5.9
1	В	595	GLU	5.3
1	В	593	ARG	5.0
1	В	386	LEU	4.6
1	В	404	THR	4.4
1	В	596	GLY	4.3
1	В	369	MET	4.3
1	В	353	ASN	4.2
1	В	389	ILE	4.1
1	В	442	PRO	4.1
1	В	402	ASN	4.1
1	В	440	VAL	4.1
1	В	414	THR	4.1
1	В	419	GLN	4.0
1	В	441	THR	4.0
1	A	331	PRO	3.9
1	В	413	PHE	3.8



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Mol	Chain	Res	Type	RSRZ
1	А	358	PHE	3.8
1	В	355	355 VAL	
1	В	592	92 PRO 3	
1	В	432	TYR	3.6
1	В	357	LEU	3.5
1	В	416	GLU	3.4
1	В	374	TYR	3.4
1	В	589	SER	3.4
1	В	367	LYS	3.3
1	А	442	PRO	3.3
1	А	317	SER	3.3
1	В	411	VAL	3.3
1	В	420	ARG	3.3
1	В	638	PRO	3.2
1	А	375	LEU	3.2
1	В	406	LEU	3.2
1	В	356	LEU	3.2
1	В	387	LEU	3.2
1	А	328	GLU	3.1
1	В	364	GLN	3.1
1	А	355	VAL	3.1
1	В	381	GLU	3.1
1	В	399	LYS	3.0
1	В	422	ALA	3.0
1	А	591	GLY	3.0
1	В	417	SER	2.9
1	А	318	ALA	2.9
1	В	358	PHE	2.9
1	В	400	PRO	2.8
1	В	426	LEU	2.8
1	В	421	GLN	2.7
1	В	597	GLY	2.6
1	В	385	GLU	2.6
1	А	332	LEU	2.6
1	А	329	GLU	2.6
1	А	426	LEU	2.5
1	В	601	GLU	2.5
1	В	378	THR	2.5
1	В	423	CYS	2.4
1	В	384	GLN	2.4
1	В	588	LYS	2.4
1	В	360	ALA	2.4



Mol	Chain	Res	Type	RSRZ
1	А	354	ALA	2.4
1	А	427	ARG	2.3
1	В	365	ASP	2.3
1	В	639	GLN	2.3
1	В	379	GLN	2.2
1	В	393	ARG	2.2
1	А	382	ASN	2.2
1	В	372	TRP	2.1
1	В	461	SER	2.1
1	В	373	GLN	2.1
1	В	520	ASN	2.1
1	А	579	PHE	2.1
1	В	434	PRO	2.1
1	А	325	GLN	2.0
1	В	383	GLU	2.0

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)

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
2	SR	В	1640	1/1	0.98	0.09	44,44,44,44	0
2	SR	A	1640	1/1	0.99	0.13	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.

