



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 05:22 AM EST

PDB ID : 1QPP
Title : CRYSTAL STRUCTURES OF SELF CAPPING PAPD CHAPERONE HOMODIMERS
Authors : Hung, D.L.; Pinkner, J.S.; Knight, S.D.; Hultgren, S.J.
Deposited on : 1999-05-28
Resolution : 2.60 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	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

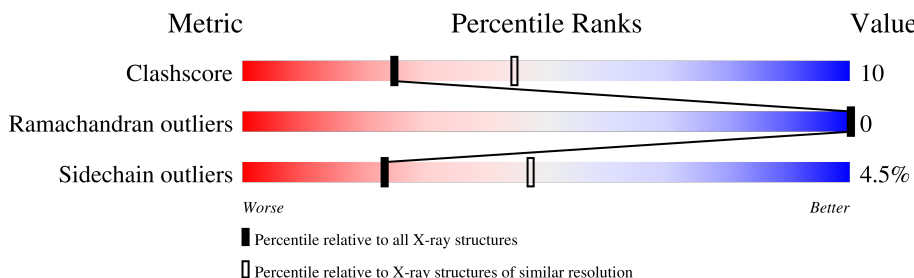
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	218	 71% 20% • 5%
1	B	218	 74% 21% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3253 atoms, of which 0 are hydrogens and 0 are deuteriums.

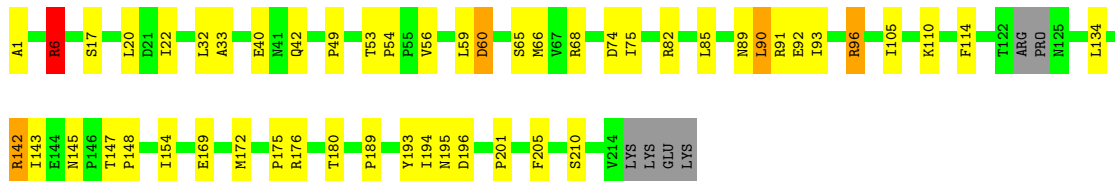
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PAPD CHAPERONE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1617	1021	276	315	5			
1	B	212	Total	C	N	O	S	0	0	0
			1636	1035	275	321	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	ARG	engineered mutation	UNP P15319
B	8	ALA	ARG	engineered mutation	UNP P15319



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.36Å 55.34Å 46.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3253	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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	A	0.54	0/1651	1.41	18/2246 (0.8%)
1	B	0.47	0/1669	1.20	9/2273 (0.4%)
All	All	0.50	0/3320	1.31	27/4519 (0.6%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH2	14.10	127.35	120.30
1	B	91	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	123	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	176	ARG	CD-NE-CZ	9.04	136.26	123.60
1	B	91	ARG	CD-NE-CZ	8.28	135.20	123.60
1	A	142	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	A	176	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	142	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	B	6	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	116	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	196	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	82	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	81	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	91	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	B	60	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	6	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	B	91	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	197	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	B	142	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	1	ALA	N-CA-CB	5.68	118.05	110.10
1	A	6	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	123	ARG	CD-NE-CZ	5.61	131.45	123.60
1	B	96	ARG	CD-NE-CZ	5.30	131.01	123.60
1	B	196	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	60	ASP	CB-CG-OD1	5.16	122.94	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	THR	CA-CB-CG2	-5.13	105.22	112.40
1	A	130	ASP	CB-CG-OD1	-5.02	113.78	118.30

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	1617	0	1588	34	0
1	B	1636	0	1600	28	0
All	All	3253	0	3188	62	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 (62) 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:137:VAL:HG12	1:A:138:SER:H	1.41	0.86
1:B:6:ARG:HD3	1:B:20:LEU:HD22	1.63	0.80
1:B:147:THR:HB	1:B:148:PRO:HD2	1.67	0.75
1:A:39:ASN:ND2	1:A:43:GLU:H	1.84	0.74
1:A:112:LYS:HD3	1:A:172:MET:HE1	1.69	0.74
1:B:42:GLN:HE21	1:B:110:LYS:NZ	1.86	0.73
1:A:32:LEU:HB2	1:A:93:ILE:HB	1.75	0.68
1:A:122:THR:HG21	1:A:128:TRP:CZ3	2.31	0.66
1:B:1:ALA:HA	1:B:92:GLU:OE1	1.99	0.62
1:A:34:GLN:NE2	1:A:93:ILE:HD11	2.16	0.61
1:A:134:LEU:HB2	1:A:212:CYS:HB2	1.82	0.61
1:B:17:SER:HB3	1:B:68:ARG:HH11	1.66	0.61
1:B:42:GLN:HE21	1:B:110:LYS:HZ2	1.48	0.60
1:B:89:ASN:OD1	1:B:110:LYS:HE2	2.02	0.60
1:A:91:ARG:HD3	1:A:106:ALA:HB1	1.85	0.58
1:A:136:LYS:HG3	1:A:210:SER:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:TYR:CZ	1:B:201:PRO:HG2	2.39	0.58
1:A:96:ARG:HH11	1:A:96:ARG:HB3	1.69	0.57
1:A:39:ASN:HD21	1:A:43:GLU:H	1.49	0.57
1:B:145:ASN:O	1:B:176:ARG:HA	2.04	0.56
1:B:189:PRO:HG2	1:B:205:PHE:HB2	1.88	0.55
1:A:193:TYR:O	1:A:200:ARG:HA	2.07	0.54
1:A:96:ARG:HH11	1:A:96:ARG:CB	2.21	0.54
1:B:147:THR:HB	1:B:148:PRO:CD	2.35	0.53
1:A:137:VAL:HG12	1:A:138:SER:N	2.17	0.53
1:B:142:ARG:HG3	1:B:180:THR:OG1	2.08	0.52
1:B:92:GLU:O	1:B:92:GLU:HG3	2.11	0.50
1:A:153:VAL:HG22	1:A:191:LEU:HD21	1.92	0.50
1:A:134:LEU:HD22	1:A:143:ILE:HG12	1.94	0.49
1:A:160:GLU:HG3	1:A:202:VAL:HG11	1.95	0.49
1:A:93:ILE:HD12	1:A:93:ILE:N	2.27	0.49
1:B:32:LEU:HB2	1:B:93:ILE:HB	1.96	0.48
1:A:34:GLN:HE21	1:A:93:ILE:HD11	1.77	0.48
1:B:40:GLU:HG3	1:B:85:LEU:HD23	1.94	0.47
1:B:42:GLN:HE21	1:B:110:LYS:HZ3	1.59	0.47
1:A:30:PRO:HB3	1:A:61:PRO:HD3	1.96	0.47
1:A:45:ILE:HD12	1:A:48:GLY:O	2.15	0.47
1:A:92:GLU:O	1:A:92:GLU:HG3	2.15	0.47
1:A:148:PRO:HD2	1:A:149:TYR:CE2	2.50	0.46
1:A:28:GLN:O	1:A:61:PRO:HG3	2.16	0.45
1:B:22:ILE:HD12	1:B:59:LEU:HD11	1.98	0.45
1:A:116:ARG:HA	1:A:117:PRO:HD2	1.80	0.45
1:B:134:LEU:CD2	1:B:143:ILE:HG12	2.46	0.45
1:B:114:PHE:HE1	1:B:172:MET:CE	2.30	0.45
1:B:33:ALA:HB1	1:B:90:LEU:HD21	1.98	0.44
1:B:193:TYR:O	1:B:201:PRO:HD2	2.17	0.44
1:A:30:PRO:O	1:A:95:PRO:HG3	2.18	0.44
1:A:34:GLN:HE22	1:A:91:ARG:HH11	1.65	0.44
1:A:81:ASP:O	1:A:148:PRO:HB3	2.18	0.44
1:B:59:LEU:HD21	1:B:65:SER:HB2	2.00	0.44
1:B:53:THR:HA	1:B:54:PRO:HA	1.84	0.43
1:A:34:GLN:HE21	1:A:93:ILE:CD1	2.30	0.43
1:B:49:PRO:HB2	1:B:75:ILE:CD1	2.49	0.42
1:A:145:ASN:OD1	1:A:147:THR:HG23	2.19	0.42
1:A:1:ALA:HA	1:A:92:GLU:OE1	2.19	0.42
1:B:68:ARG:HH11	1:B:68:ARG:HG3	1.85	0.42
1:B:154:ILE:HG21	1:B:194:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASN:HD22	1:B:201:PRO:HD3	1.85	0.41
1:B:148:PRO:C	1:B:175:PRO:HB3	2.40	0.41
1:A:6:ARG:HD3	1:A:20:LEU:HD22	2.03	0.41
1:A:134:LEU:HD23	1:A:143:ILE:HG23	2.03	0.41
1:A:137:VAL:CG1	1:A:138:SER:H	2.22	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	203/218 (93%)	194 (96%)	9 (4%)	0	100	100
1	B	208/218 (95%)	200 (96%)	8 (4%)	0	100	100
All	All	411/436 (94%)	394 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	178/193 (92%)	173 (97%)	5 (3%)	38	65
1	B	179/193 (93%)	168 (94%)	11 (6%)	15	34
All	All	357/386 (92%)	341 (96%)	16 (4%)	23	47

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	39	ASN
1	A	70	SER
1	A	96	ARG
1	A	147	THR
1	B	6	ARG
1	B	56	VAL
1	B	60	ASP
1	B	66	MET
1	B	74	ASP
1	B	82	ARG
1	B	90	LEU
1	B	96	ARG
1	B	105	ILE
1	B	169	GLU
1	B	210	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	39	ASN
1	A	42	GLN
1	B	41	ASN
1	B	42	GLN
1	B	187	ASN
1	B	195	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.