



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 PM GMT

PDB ID : 4RHP  
Title : Crystal structure of human COQ9 in complex with a phospholipid, Northeast Structural Genomics Consortium Target HR5043  
Authors : Forouhar, F.; Lew, S.; Seetharaman, J.; Wang, H.; Lee, D.; Kogan, S.; Maglaqui, M.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG); Mitochondrial Protein Partnership (MPP)  
Deposited on : 2014-10-02  
Resolution : 2.39 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

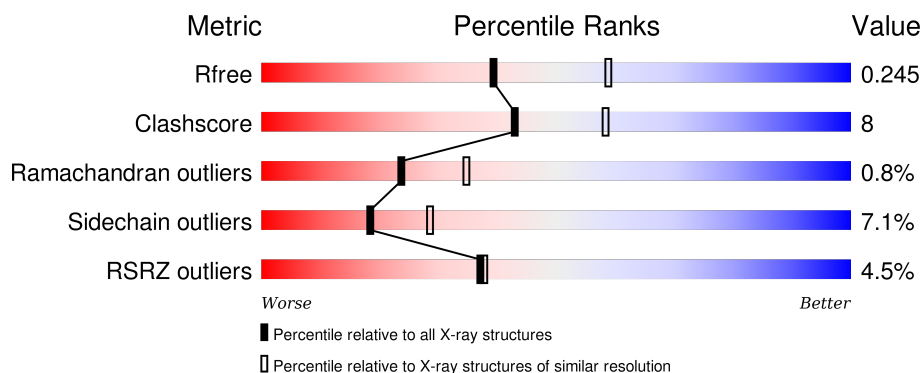
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	235	
1	B	235	

## 2 Entry composition [i](#)

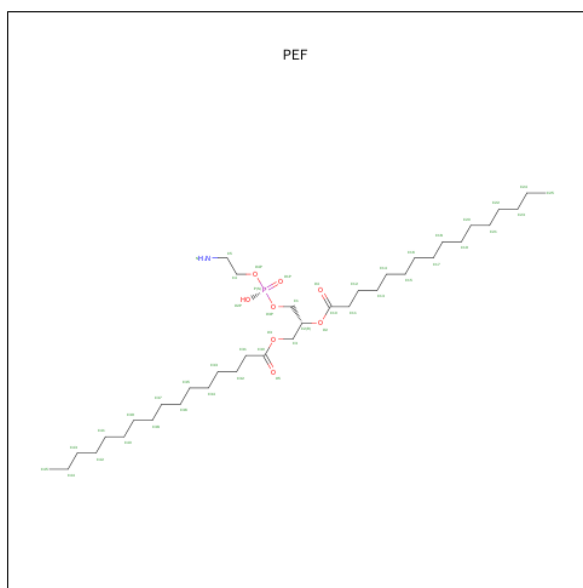
There are 3 unique types of molecules in this entry. The entry contains 3281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ubiquinone biosynthesis protein COQ9, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	Se	0	0	0
			1517	954	263	289	1	10			
1	B	207	Total	C	N	O	S	Se	0	0	0
			1642	1036	283	311	1	11			

- Molecule 2 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			32	23	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	31	Total	O	0	0
			31	31		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.34Å 97.63Å 64.11Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	48.79 – 2.39 48.81 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.79-2.39) 99.4 (48.81-2.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.39Å)	Xtriage
Refinement program	XtalView and PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.179 , 0.246 0.179 , 0.245	Depositor DCC
$R_{free}$ test set	1885 reflections (11.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18457 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PEF

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	0.47	0/1539	0.58	0/2070
1	B	0.39	0/1662	0.51	0/2231
All	All	0.43	0/3201	0.55	0/4301

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

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	1517	0	1476	15	0
1	B	1642	0	1610	39	0
2	A	32	0	37	0	0
3	A	59	0	0	0	0
3	B	31	0	0	2	0
All	All	3281	0	3123	52	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 8.

All (52) 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:121:ILE:HD11	1:B:145:LEU:HB2	1.57	0.87
1:B:201:PRO:HG3	1:B:259:MSE:HG3	1.58	0.86
1:A:281:MSE:HA	1:A:281:MSE:HE3	1.63	0.81
1:B:147:LEU:O	1:B:151:THR:HG23	1.85	0.76
1:B:118:ALA:HB2	1:B:140:LYS:HA	1.70	0.72
1:B:264:PRO:O	1:B:267:GLU:HG3	1.91	0.71
1:B:282:ASN:O	1:B:283:MSE:HB2	1.92	0.70
1:B:183:ARG:CZ	1:B:274:GLU:HG3	2.22	0.69
1:B:275:ASN:HD22	1:B:293:THR:HG21	1.58	0.69
1:B:111:VAL:N	1:B:112:PRO:HD2	2.09	0.68
1:B:255:GLU:O	1:B:259:MSE:HE2	1.97	0.65
1:B:310:ASN:O	1:B:311:LEU:HB2	1.97	0.63
1:B:118:ALA:HB3	1:B:140:LYS:HD2	1.81	0.62
1:A:138:PHE:HB3	1:A:144:GLU:OE2	1.99	0.62
1:B:137:MSE:HG3	1:B:138:PHE:CD2	2.35	0.61
1:B:108:LEU:HD13	1:B:145:LEU:HD11	1.83	0.60
1:A:108:LEU:HD13	1:A:145:LEU:HD11	1.83	0.60
1:B:137:MSE:HG3	1:B:138:PHE:CE2	2.37	0.59
1:A:99:LEU:HD23	1:A:102:ARG:HH12	1.69	0.58
1:A:281:MSE:HA	1:A:281:MSE:CE	2.34	0.57
1:A:99:LEU:HD23	1:A:102:ARG:NH1	2.20	0.56
1:A:122:ALA:O	1:A:126:GLN:HG3	2.06	0.55
1:B:101:HIS:HD2	3:B:413:HOH:O	1.91	0.54
1:A:147:LEU:O	1:A:151:THR:HG22	2.07	0.54
1:A:233:ASP:O	1:A:236:THR:HG22	2.08	0.54
1:B:118:ALA:CB	1:B:140:LYS:HA	2.36	0.53
1:A:147:LEU:O	1:A:151:THR:CG2	2.60	0.49
1:A:165:GLN:O	1:A:169:GLN:HG3	2.12	0.48
1:A:208:MSE:SE	1:B:301:LEU:HD21	2.65	0.47
1:B:111:VAL:N	1:B:112:PRO:CD	2.78	0.47
1:B:272:PHE:CD1	1:B:293:THR:HB	2.50	0.46
1:A:122:ALA:HB1	1:A:132:SER:HB2	1.97	0.46
1:B:240:TRP:CZ3	1:B:241:TYR:HD1	2.34	0.46
1:B:276:ARG:HH22	1:B:293:THR:CB	2.30	0.45
1:B:125:ALA:O	1:B:130:LEU:HB2	2.16	0.45
1:B:121:ILE:CD1	1:B:145:LEU:HD22	2.47	0.45
1:B:275:ASN:HD22	1:B:293:THR:CG2	2.27	0.44
1:B:276:ARG:HH22	1:B:293:THR:HB	1.80	0.44
1:B:183:ARG:HG3	1:B:277:VAL:HG21	1.99	0.44
1:B:311:LEU:HD22	1:B:311:LEU:HA	1.87	0.44
1:B:239:ASN:HD21	1:B:241:TYR:HB3	1.82	0.44
1:B:121:ILE:HD13	1:B:145:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:HIS:CD2	1:B:148:HIS:HE1	2.36	0.43
1:B:139:GLY:C	1:B:141:ASP:H	2.22	0.43
1:B:190:LEU:O	1:B:193:LEU:HB2	2.19	0.43
1:B:139:GLY:O	1:B:141:ASP:N	2.52	0.42
1:B:111:VAL:O	1:B:113:ALA:N	2.54	0.41
1:B:228:TRP:CE2	1:B:243:ARG:HB3	2.56	0.41
1:B:101:HIS:CD2	3:B:413:HOH:O	2.69	0.41
1:A:267:GLU:HG2	1:A:271:ARG:HH12	1.85	0.41
1:A:283:MSE:HB3	1:B:211:HIS:HB3	2.02	0.40
1:B:205:SER:HB3	1:B:308:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	187/235 (80%)	182 (97%)	5 (3%)	0	100	100
1	B	201/235 (86%)	193 (96%)	5 (2%)	3 (2%)	13	17
All	All	388/470 (83%)	375 (97%)	10 (3%)	3 (1%)	24	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	283	MSE
1	B	137	MSE
1	B	140	LYS

### 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	164/188 (87%)	152 (93%)	12 (7%)	17	27
1	B	175/188 (93%)	163 (93%)	12 (7%)	19	30
All	All	339/376 (90%)	315 (93%)	24 (7%)	18	28

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	108	LEU
1	A	130	LEU
1	A	140	LYS
1	A	143	SER
1	A	151	THR
1	A	204	LEU
1	A	207	LEU
1	A	209	LEU
1	A	233	ASP
1	A	281	MSE
1	A	283	MSE
1	B	108	LEU
1	B	141	ASP
1	B	151	THR
1	B	179	ASP
1	B	193	LEU
1	B	204	LEU
1	B	209	LEU
1	B	213	ILE
1	B	256	LEU
1	B	259	MSE
1	B	298	VAL
1	B	311	LEU

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

Mol	Chain	Res	Type
1	A	98	GLN
1	A	100	GLN
1	A	169	GLN
1	A	234	GLN
1	B	148	HIS
1	B	172	GLN
1	B	275	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 carbohydrates 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	$\# Z  > 2$
2	PEF	A	401	-	31,31,46	1.62	5 (16%)	34,36,51	1.35	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEF	A	401	-	-	0/33/33/50	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PEF	C32-C31	-4.77	1.34	1.52
2	A	401	PEF	C36-C35	-3.03	1.34	1.51
2	A	401	PEF	C37-C36	-2.38	1.33	1.51
2	A	401	PEF	O2-C10	4.01	1.46	1.34
2	A	401	PEF	O3-C30	4.20	1.46	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PEF	C2-O2-C10	-2.09	112.88	117.89
2	A	401	PEF	O3-C30-O5	-2.08	118.12	123.49
2	A	401	PEF	C32-C31-C30	2.25	122.44	113.59
2	A	401	PEF	O3-C30-C31	2.77	120.34	111.90
2	A	401	PEF	O2-C10-C11	3.83	119.86	111.53

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	179/235 (76%)	0.18	7 (3%) 43 44	16, 34, 69, 121	0
1	B	196/235 (83%)	0.37	10 (5%) 32 32	25, 43, 85, 100	0
All	All	375/470 (79%)	0.28	17 (4%) 37 38	16, 38, 83, 121	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	THR	4.8
1	B	133	ALA	4.4
1	A	235	SER	3.9
1	B	132	SER	3.9
1	B	172	GLN	2.9
1	B	140	LYS	2.8
1	A	95	SER	2.5
1	B	311	LEU	2.4
1	A	234	GLN	2.4
1	A	97	GLU	2.3
1	B	174	GLU	2.3
1	B	93	TYR	2.2
1	A	144	GLU	2.2
1	B	163	GLU	2.2
1	A	152	GLN	2.0
1	A	233	ASP	2.0
1	B	138	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEF	A	401	32/47	0.92	0.18	1.67	53,64,83,87	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.